Final Project Report

Design of Catalytic Monoliths for Closed-Cycle Carbon Dioxide Lasers

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Submitted by

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*Each section pages individually numbered.

Abstract

Pulsed carbon dioxide (CO_2) lasers have many applications in aeronautics, space research, weather monitoring and other areas. Full exploitation of the potential of these lasers is hampered by the dissociation of CO_2 that occurs during laser operation. The development of closed-cycle CO_2 lasers require active CO-O_2 recombination (CO oxidation) catalyst and design methods for implementation of catalysts in CO_2 laser systems.

A monolith catalyst section model and associated design computer program, LASCAT, are presented to assist in the design of a monolith catalyst section of a closed cycle CO_2 laser system. Using LASCAT, the designer is able to specify a number of system parameters and determine the monolith section performance. Trade-offs between the catalyst activity, catalyst dimensions, monolith dimensions, pressure drop, O_2 conversion, and other variables can be explored and adjusted to meet system design specifications.

An introduction describes a typical closed-cycle CO_2 system, and indicates some advantages of a closed-cycle laser system over an open cycle system and some advantages of a monolith support over other types of supports. The development and use of a monolith catalyst model is presented. The results of a design study and a discussion of general design rules are given. Detailed instructions for the use of LASCAT is given in Appendices 1-4.

Monolith Catalyst Model Development and Implementation

1. INTRODUCTION

The design of a CO_2 laser system is made under constraints of energy consumption, operating cost, size, weight, pressure drop, loop O_2 conversion, catalyst activity, flow channel dimensions, particulate production, reliability, ease of operation, safety, and numerous others. Design decisions, made to satisfy one constraint, often push the limits imposed on other constraints. A means to design the monolith catalyst section of a closed-cycle CO_2 laser system under selected restraint conditions is presented.

A pulsed CO_2 laser produces useful laser light output when the laser gas volume is exposed to a high electrical potential for a period on the order of milliseconds [1,2]. Low lying vibrational-rotational energy level CO_2 molecules are excited to higher energy levels. The relaxation of the excited molecules to low lying energy levels produces infrared radiation ($\approx 10\mu m$). The energy deposited by the electrical discharge alters the composition of the gas mixture by dissociation of CO_2 into stoichiometric ratios of CO and O_2. In a high pulse repetition rate (PRR) CO_2 laser system, without a method of recombining the CO and O_2, the laser gas O_2 concentration would continue to increase with time. Depending on the particular system used, O_2 concentrations above a threshold level, on the order of 1%, severely degrades the laser output quality. The lasing process also raises the temperature of the laser gas volume. The output of the laser is sensitive to the temperature of the operating gas due to the effect of temperature on the distribution of CO_2 molecules among the rotational-vibrational energy levels.

An open-cycle laser system requires a continuous supply of fresh gas to maintain O_2 concentration below threshold levels. The higher the PRR, the higher the fresh gas flow rate required to maintain acceptable O_2 concentrations. If rare isotope CO_2 gases[1,3], such as $^{12}C^{18}O_2$, were to be used in an open-cycle laser system, the cost of supplying large quantities of CO_2 gases would be prohibitive. The safety requirements for handling and for the disposal of CO, O_2, and CO_2 gases is another concern for open-cycle systems. Clearly, for portable uses, such as in satellites or in the field, open-cycle system operation is not feasible.

Closed-cycle systems can be envisioned to require an one time charge of the operating gas and to operate for a given number of pulses ($>10^7$) at a specified PRR and power output[4-7]. Portable closed-cycle systems would necessarily have power consumption constraints and, therefore, be limited in the output power and PRR. In a typical closed-cycle CO_2 laser system (Fig. 1), a gas mixture, comprised of CO_2 and other "inert" gases, is continuously recirculated through the system by a blower. The recombination of CO and O_2 is accomplished by the monolith catalyst section of the system (Fig. 2) and provides the laser section with a fresh supply of operating gas. The heat exchangers allow for the operation of the monolith catalyst section at elevated temperatures while maintaining moderate laser section temperatures. The monolith catalyst material is very porous (high surface area) and has catalytic material dispersed throughout. The performance of the monolith catalyst is measured by the section's ability to recombine CO and O_2, the size and weight of the monolith, and the pressure drop produced as a result of gas flow through the monolith. Monolith catalyst performance is dependent on a number of interrelated factors, such as, the catalyst's geometry, convective heat and mass transport rates from the bulk gas to the catalyst, inlet gas properties, inlet molar gas flow rate, and catalytic activity. A monolith support is chosen over other supports, e.g. powders, beads, etc., because of the reduced level of particulate production, and the sturdiness of the monolith under high volumetric gas flow conditions.

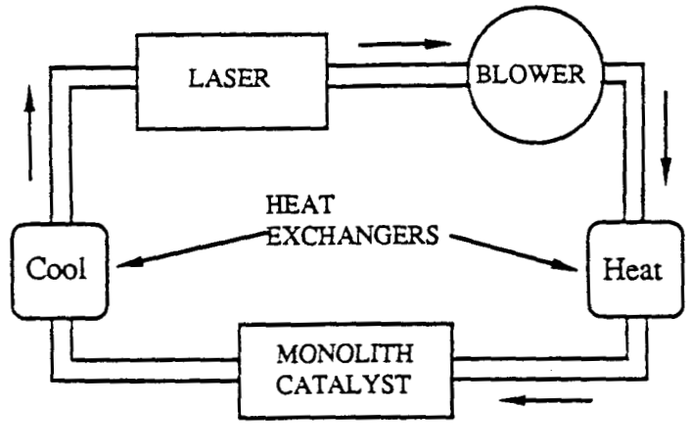

Figure 1. A typical closed-cycle CO_2 laser.

2. MONOLITH CATALYST SECTION MODEL

A flexible model of the monolith catalyst may be developed to determine the bulk-average gas temperature, composition, and pressure along the length of the monolith. The adjustable parameters required to specify the operating condition of the monolith are listed in Table 1. The model assumptions, balance equations, and model results follow.

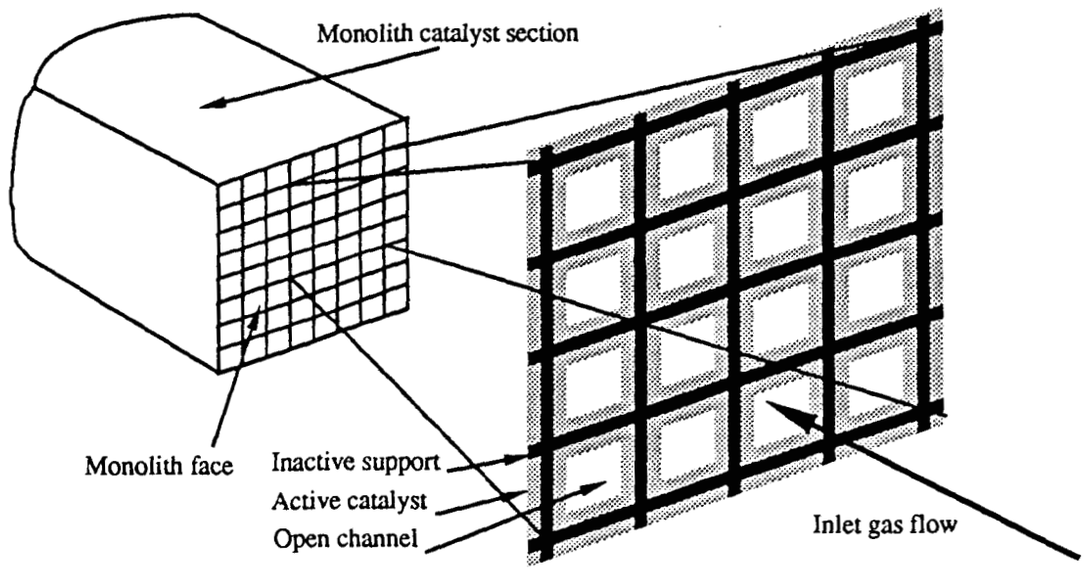

Figure 2. Monolith catalyst section.

2.1 Model Assumptions

- Steady state conditions.
- Identical conditions exist in each channel of the monolith.

•Channel gas flow is laminar and fully developed. The neglect of entrance effects for heat and mass transfer calculations provide for a conservative estimate of the amount of catalyst required. Pressure drop due to entrance and exit effects is neglected, therefore the actual pressure drops will be somewhat greater than calculated.
•The kinetics of the reaction, $^1/_2O_2 + CO \rightarrow CO_2$, is first order overall, reaction rate $\propto [O_2]^a [CO]^b$ where sum of a and b equals one. O_2 and CO_2 appear in stoichiometric ratios, 2:1≡ CO:O_2. The concentration of O_2 is followed and the remaining species concentrations are calculated. The effect of temperature on the reaction rate is through an Arrhenius dependence of a reaction rate constant.
•Inlet gas composition, temperature and flow rate are known. Gas properties, viscosity, diffusivity, and thermal conductivity, are updated with changes in temperature, pressure, and reactant concentrations.
•Diffusivity in the porous catalytic layer is calculated using size and void fraction of micropores and macropores. Equimolar counterdiffusion in porous catalytic layer is assumed.
•Either adiabatic or isothermal monolith operating conditions can be selected by the operator. These two operating conditions provide the upper and lower bounds for oxygen conversion for a given inlet gas condition.
• Axial heat conduction in the porous catalytic layer and support is assumed to be negligible. For adiabatic monolith operation, transverse heat conduction the porous catalytic layer and support is assumed to be such that the porous catalytic layer and support temperature is uniform transversely.
•Slab geometry is used for calculation of the species concentration in the porous catalytic layer. A characteristic porous catalytic layer thickness is calculated to account for porous catalytic material in the channel corners.
•Heat and mass transport between the flowing gas and the channel walls are described using the limiting Sherwood (Sh_∞) and Nusselt (Nu_∞) numbers for constant wall concentration and temperature boundary conditions in square channels[8].

2.2 Model balance equations

The steady state conservation equations for O_2 in the flowing gas and O_2 in the porous catalytic layer are

$$\frac{d\Phi_G}{d\zeta} = -\frac{\gamma}{\Gamma}\left[\Phi_G - \Phi_W\right] \quad , \text{and} \quad \frac{d^2\Psi}{d\lambda^2} = \varphi^2 \Psi \quad , \tag{1,2}$$

with initial and boundary conditions,

$$\Phi_G = 1 \text{ at } \zeta = 0 \quad , \quad \Psi = 1 \text{ at } \lambda = 0 \text{ for all } \zeta \quad , \text{and} \quad \frac{d\Psi}{d\lambda} = 0 \text{ at } \lambda = 1 \quad . \tag{3,4,5}$$

Φ_G is the dimensionless bulk-average O_2 molar flow rate in the flowing gas. Variables and parameters are defined in detail in the notation list. Φ_W is the O_2 concentration at the channel wall times bulk-average volumetric flow rate divided by the inlet bulk-average O_2 molar flow rate. [$\Phi_G - \Phi_W$] is proportional to the concentration driving force for transport of O_2 from the flowing gas to the channel wall. ζ is the dimensionless distance down the length of the monolith. Ψ is the dimensionless O_2 concentration inside the porous catalytic layer at a dimensionless depth λ into the layer. The solution to equation (2) yields an overall O_2 reaction rate in the porous catalytic layer as a function of Φ_W. At steady state, this reaction rate is equal to the rate of transport of O_2 from the flowing gas to the channel wall, and leads to

$$\Phi_W = \Phi_G \left[\frac{1}{\alpha + 1}\right] \quad . \tag{6}$$

The steady state energy balance on the flowing gas relates the rise in the dimensionless bulk-average temperature of the flowing gas, θ_G, to the heat transferred to the gas from the channel wall and yields

$$\frac{d\theta_G}{d\zeta} = -\left[\frac{d_h S\, St}{\Gamma}\right]\left[\theta_G - \theta_W\right] \quad , \text{ with initial condition, } \quad \theta_G = 1 \text{ at } \zeta = 0 \quad , \quad (7,8)$$

where θ_G is the dimensionless bulk-average temperature of the flowing gas, and θ_W is the dimensionless temperature at the channel wall. An energy balance on the porous catalytic layer equates the heat generation from the oxygen consumption reaction to the heat transferred from the porous catalytic layer and yields

$$-\left[\frac{\omega\,\alpha}{\Gamma}\right]\Phi_W = \left[\theta_G - \theta_W\right] \quad . \quad (9)$$

Combining the two energy balance equations, (7) and (9), and substituting for Φ_W using equation (6) results in two final differential equations, to be integrated,

$$\frac{d\Phi_G}{d\zeta} = -\left[\frac{\Gamma}{\gamma} + \frac{\Gamma}{\alpha\gamma}\right]^{-1}\Phi_G \quad , \text{and} \quad \frac{d\theta_G}{d\zeta} = \frac{[d_h S\,\alpha\,\omega\,St]}{[1+\alpha]\,\Gamma^2}\Phi_G \quad , \quad (10,11)$$

with the same initial conditions for Φ_G and θ_G as above. Pressure drop for the laminar flow is calculated using the Hagen-Poiseuille equation,

$$\frac{d\wp}{d\zeta} = \frac{-32}{Eu\,Re} \quad , \text{ with an initial condition of } \quad \wp = 1 \text{ at } \zeta = 0 \quad , \quad (12,13)$$

where $\wp$ is the dimensionless pressure. Equations (10), (11), and (12) are coupled to each other through the variable Φ_G and the parameters α, ω, Γ, γ, St, Eu, and Re, each of which is a function of θ_G, Φ_G and $\wp$.

2.3 Model results

The adjustable parameters required to specify the monolith catalyst section operating conditions are listed below in Table 1. They are used to compute the dimensionless parameters α, ω, Γ, γ, St, Eu, and Re, and to integrate the dimensionless variables in equations (10), (11), and (12). A computer program (see section 5) was written to perform integration using fourth order Runge-Kutta method. The program outputs θ_G, θ_W, Φ_G, Φ_W and $\wp$ as ζ varies from zero to the desired dimensionless monolith catalyst section length. The computer program requires readily available parameters to calculate parameters such as mass and heat transfer coefficients, bulk-gas and effective diffusion coefficients, and thermal conductivity. Results for a monolith catalyst section operating under conditions specified in Table 1 are shown in Figs. 3, 4 and 5.

Fig. 3 shows the behavior of θ, Φ , and $\wp$ as ζ varies from 0 to 100. $\theta_G \approx \theta_W$ and $\Phi_G \approx \Phi_W$, therefore θ_G, θ_W, Φ_G, and Φ_W are not shown individually on this small scale plot. The behavior of θ, Φ, and $\wp$ can be explained using equations (1)-(12), in which all parameters and variables are positive valued. The right side of equation (11) is positive, therefore, $d\theta_G/d\zeta > 0$. The left hand side of equation (9) is negative, therefore, $\theta_W > \theta_G$. Similar examination of equations (10) and (6) results in $d\Phi_G/d\zeta < 0$ and $\Phi_W > \Phi_G$. Equation (12) indicates that $d\wp/d\zeta < 0$. The drop in $\wp$ is negligible for the gas flow rate specified in Table 1. Pressure drop can be significant for higher gas flow rates.

Fig. 4 is an expansion of Fig. 3 in the ζ = 45 to 50 region. The separation between θ_G and θ_W is now visible and provides an indication of the thermal driving force between the channel wall and the bulk-gas. Heat produced from the oxidation of CO in the active catalyst layer of the channel wall is transferred from the channel wall to the bulk-gas.

Fig. 5 is also an expansion of Fig. 3 in the ζ = 45 to 50 region. An additional curve, $\Psi(\lambda=1)*\Phi_W$, is the scaled O_2 concentration at the centerline of the monolith channel support wall. O_2 is consumed in the porous catalytic layer as mass transport to the center of the monolith channel support wall occurs,

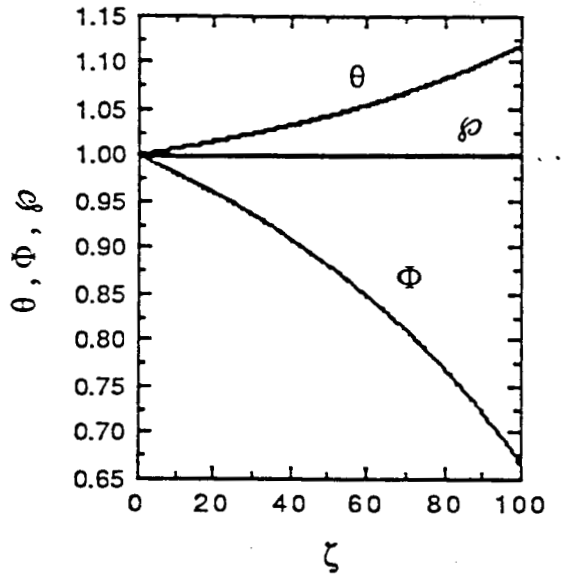

Figure 3. Results for Table 1 case. Dimensionless bulk-gas temp (θ), pressure (℘), and O_2 concentration (Φ) vs distance from mono-inlet (ζ).

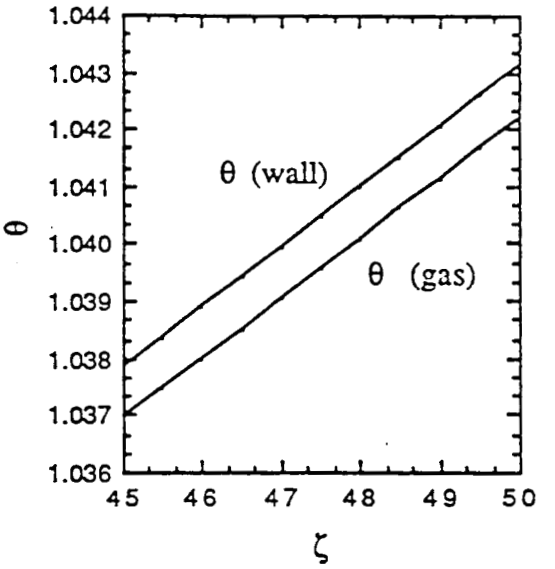

Figure 4. Dimensionless temperatures for Table 1 case.

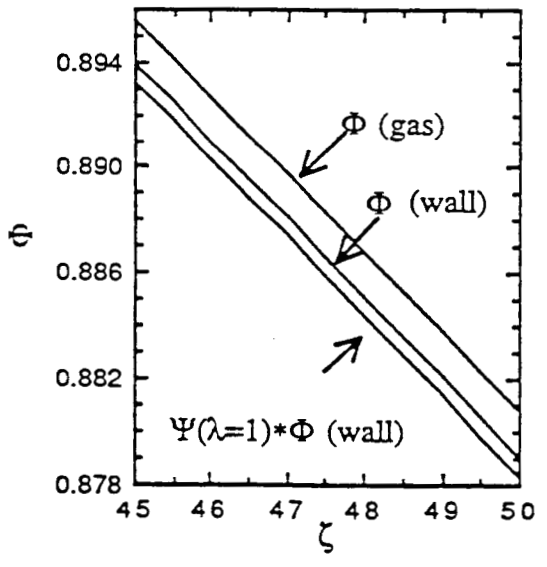

Figure 5. Dimensionless O_2 concentrations for Table 1 case.

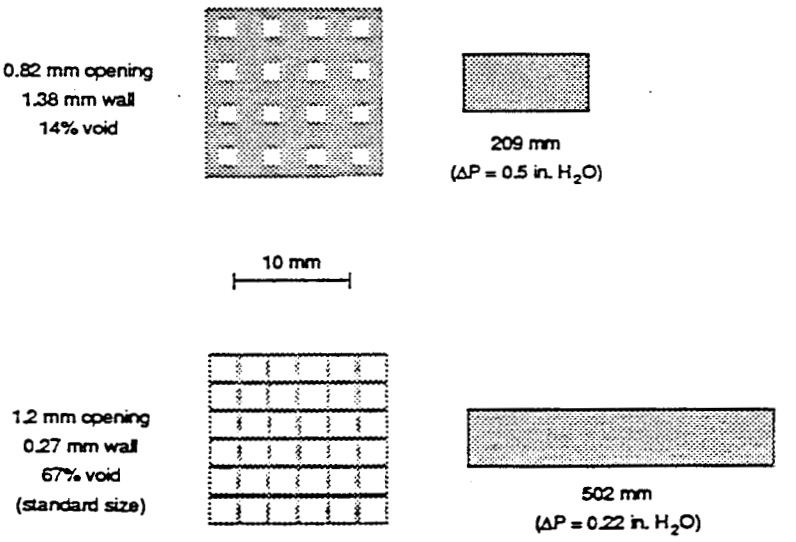

Figure 6. Optimum design vs. standard commercial size.

therefore $\Psi(\lambda=1)*\Phi_W$ is less than Φ_W or Φ_G. The separation between the curves indicates the O_2 mass transport driving force. The difference between Φ_G and Φ_W is an indication of the driving force between the bulk gas and the channel wall. The difference between Φ_W and $\Psi(\lambda=1)*\Phi_W$ is an indication of the driving force between the channel wall and the centerline of the monolith channel support wall.

Table 1: Monolith catalyst section operating parameters

Monolith dimension	Catalyst properties
Facial cross sectional area = 1.0e+4 mm^2	Void fraction as macropores = 0.25
Support wall thickness(including active layer) = 1mm	Void fraction as micropores = 0.48
Active layer thickness = 0.25mm	Macropore radius = 500nm
Gas inlet properties	Micropore radius = 12nm
Flowrate = 0.25 liters/sec	Active layer density = 0.5e-3 g/mm^3
Temperature = 300 K	Reaction rate constant = 123.4mm^3/gcat sec (at 298K)
Pressure = 101.325 kPa	Activation energy constant = 39700 J/mol
Composition 37% CO_2, 2% CO, 1% O_2 40% N_2, 20% He	
Thermal operation is adiabatic.	

3. DESIGN STUDY

3.1 Design constraints

A design study for a monolith catalyst section, operating under parameters similar to those listed in Table 1, was performed. For the study, the support wall was assumed to be composed entirely of active catalytic material. Additional constraints, 25% O_2 conversion (Φ_G[exit]=0.75) and a 0.125kPa (≈0.5 in H_20) pressure drop across the monolith section, were imposed. The monolith facial cross sectional area and inlet gas conditions (composition, temperature, flow, and pressure) were held constant. Active support wall thickness and channel opening dimensions were varied and the minimum monolith length determined under the imposed constraint conditions.

The rationale for minimizing the monolith length follows from the assertion that the smallest monolith leads to the smallest, lightest and least expensive laser system. In portable laser systems size, weight, and cost considerations are critical. The choice of the shortest monolith section reduces the system weight by reducing the required monolith section housing length. The housing material weight per unit length is typically an order of magnitude more than that of the monolith material. The monolith material can be quite expensive; a smaller system requires less materials and is less costly. The 25% conversion requirement ensures a constant gas temperature rise. A constant pressure drop across the monolith section ensures that an identical amount of energy is expended to circulate the gas through the system. Excluding laser pulse energy, system energy requirements (blower energy and heating and cooling loads) are fixed by the pressure drop and conversion requirements. Constant gas inlet conditions and 25% conversion ensure that a chosen laser PRR can be maintained without exceeding a the maximum allowable laser section inlet O_2 concentration.

3.2 Design results

Fig. 6 shows the optimum monolith section design geometry in comparison with a standard monolith design. The optimum monolith length is substantially less than the standard monolith length, whereas the optimum support wall thickness is substantially greater than standard thickness. As the monolith support wall thickness is increased, more catalytic material can be packed into a shorter monolith while conversion and pressure drop constraints are still satisfied. However, a thicker support wall has a larger O_2 mass transport resistance. A point is reached where the benefit of having thicker walls is negated by the large O_2 mass transport resistance and an optimum monolith length is determined.

4. DISCUSSION

The design study presented above shows that the use of off-the-shelf commercial monolith designs for CO_2 laser applications dramatically increases the overall monolith size required relative to the optimum design presented here. Off-the-shelf monoliths are designed for pollutant emission control and have been optimized for large gas flows and fast reactions at high temperatures. They have relatively thin monolith catalyst section dimensions and high % void volume. The slow reaction rates obtained over laser catalysts allow use of relatively thick monolith wall dimensions. With lower gas flow rates, low % void volume can be used to obtain compact monoliths, thereby reducing the size, weight, and cost of the laser system.

Using a computer program to generate variable and parameter values along the length of the monolith allows for rapid optimization of monolith section under a set of constraints. Use of a computer program also allows for complex channel geometries, such as cylindrical, hexagonal, triangular, etc., to be incorporated into the monolith design.

5. MODEL IMPLEMENTATION USING LASCAT

LASCAT, a computer program based on the monolith catalyst section model presented above, provides a means to design a monolith catalyst section that will satisfy a user specified set of design requirements. LASCAT requires the specification of the parameters listed in Table 1 and an few others. Values of key parameters (Re, C_{PG}, ρ_g, D_{AB}, D_{ABeff}, and mole fractions) are provided at the inlet and exit of the monolith section. F_G, T and P are integrated instead of the corresponding nondimensional parameters, Φ_G, θ_G and $\wp$. C, T and P values are provided along the length monolith. See Appendix 2, a step by step tutorial, for an example of the LASCAT output .

Appendix 1 gives detailed information on the implementation and compatibility of LASCAT. Appendix 3 details each menu operation of LASCAT. Appendix 4 is a program listing of LASCAT and provides a wealth of information on program structure, variable definitions and units, and physical properties computational methods and references.

6. NOTATION LIST

6.1 Variables and parameters

A = CO oxidation reaction rate constant (mm^3 / g-cat s)
C = concentration of oxygen (mol / mm^3)
C_{PG} = bulk-average gas heat capacity (J / g K)
D_{AB} = diffusion constant for O_2 in bulk gas mixture (mm^2 / s)
D_{ABeff} = effective diffusion constant for oxygen in porous catalytic layer (mm^2 / s)
d_h = hydraulic diameter of monolith channel, 4(cross sectional area)/(wetted perimeter) (mm)
Eu = Euler number, $Eu = P_0 d_h^4 / \upsilon^2 \rho_g$
F_G = bulk-average gas molar flow rate of oxygen, $F_G = C_G \upsilon$ (mol / s)
h = average heat transfer coefficient (W / mm^2 K)
ΔH_{rxn} = heat of CO oxidation reaction (J / mol O_2 converted)
k = bulk-average gas thermal conductivity (J / m K)
k_m = average mass transfer coefficient (mm / s)
Nu_∞ = limiting Nusselt number, $Nu_\infty = h d_h / k$
P = pressure in the channel at a position ζ (kPa)
$\wp$ = dimensionless pressure at position ζ, $\wp = P / P_0$
Re = Reynolds number , $Re = d_h \upsilon \rho_g / \mu_g d_h^2$
S = Surface area of the channel wall per unit open volume of monolith channel (mm^2/ mm^3)
Sh_∞ = limiting Sherwood number, $Sh_\infty = k_m d_h / D_{AB}$
St = Stanton number , $St = h d_h^2 / \upsilon_0 \rho_g C_{PG}$
t_c = characteristic thickness of porous catalytic layer (mm)

6.2 Subscripts

C,c in porous catalytic layer
G,g in flowing gas
O,o at inlet conditions
W,w in gas at channel wall

T = temperature (K)
x = distance along the length of the monolith channel (mm)
z = depth into the porous catalytic layer (mm)

Greek
α = dimensionless rate constant, $\alpha = t_c \rho_c \eta A / k_m$
γ = dimensionless mass transfer coefficient, $\gamma = d_h S k_m d_h^2 / \upsilon_0$
Γ = dimensionless volumetric flow rate, $\Gamma = \upsilon / \upsilon_0$
ω = dimensionless heat of reaction, $\omega = -\Delta H_{rxn} k_m F_{G0} / h T_{G0} \upsilon_0$
ζ = dimensionless distance along the length of the monolith channel, $\zeta = x / d_h$
η = effectiveness factor of the reaction in the monolith porous catalytic layer , $\eta = \tanh(\varphi) / \varphi$
θ = dimensionless bulk gas temperature, $\theta_G = T_G / T_{G0}$, $\theta_W = T_W / T_{G0}$
λ = dimensionless depth into the porous catalytic layer, $\lambda = z / t_c$
μ_g = viscosity of gas in channel (Pa-s)
ρ_c = density of porous catalytic layer material (g-cat / mm^3)
ρ_g = density of flowing gas (g / mm^3)
υ = volumetric flow rate of flowing gas (mm^3 / s)
Φ_G = dimensionless bulk-average oxygen concentration in flowing gas, $\Phi_G = F_G / F_{G0}$
Φ_W = dimensionless channel wall surface oxygen concentration, $\Phi_W = [C_W(\zeta)\, \upsilon(\zeta)] / F_{G0}$
φ = Thiele modulus, $\varphi^2 = [t_c^2 \rho_c \eta A] / D_{ABeff}$
Ψ = dimensionless O_2 concentration in the porous catalytic layer. $\Psi(\lambda) = [C_C(\lambda) / C_W(\zeta)]$

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Appendix 1: Program Implementation and Compatibility

The LASCAT program is written in the FORTRAN programming language and is compatible with FORTRAN 77 standards. Detailed implementation instructions are provided below for Apple Macintosh and Digital Equipment Corporation VAX computers. Familiarity with the particular operating system is assumed.

Computer: Apple Macintosh SE or II.
Operating System: Apple System Version 6.0
Application Program: Absoft's MacFortran/020 Version 2.3
Compilation Options (Macintosh SE):
-Use compilation options B (Compile Using Long Addresses)
E (Generate Errors List), and
U (* = Unit 9).
Compilation Options (Macintosh II):
-Use compilation options B (Compile Using Long Addresses),
E (Generate Errors List),
M (68020/68030 instructions),
P (68881/68882 instructions), and
U (* = Unit 9).
Compilation and Execution:
-Place the LASCAT program in the same folder as the MacFortran/020 application and supporting files.
-Double click on MacFortran/020 application to launch the MacFortran/020 application.
-From the File Menu choose the "Select File" option. Select File LASCAT.
-From the Compile Menu choose the "Options" option and verify the compilation options selected are identical to the compilation options described above. If the options selected need to be changed, remember to save the new set of compilation options by clicking on the "Save" box. Exit the compilation options section by clicking on the "OK" box.
-From the Compile Menu choose the "Compile and Execute" option. The program will be compiled and executed. The output file, LDATA, and any selectable parameter files will be placed in the same folder as the LASCAT and MacFortran/020 files.

Computer: Digital Equipment Corporation VAX 11/780
Operating System: VAX/VMS Version 4.6
Application Program: VAX FORTRAN V4.8-276
Compilation and Execution :
-Rename the LASCAT program *LASCAT.for*
-To compile LASCAT.for, type *for LASCAT.for*
-To link LASCAT.for type *link LASCAT*
-To execute LASCAT.for *type run LASCAT*
-The output file, LDATA.DAT, and any selectable parameter files will be placed in the your directory. Use an editing program to examine files.

Appendix 2: LASCAT Tutorial

The LASCAT Tutorial provides a step by step example of the use of the program LASCAT. Required user input and comments are detailed on the left margin and the corresponding screen outputs are indented. Input(s) required by the operater are boldfaced. The example shown below was run on a Macintosh II using Absoft's MacFortran/020 Version 2.3 (Review the Program Implementation and Compatibility section for program complilation and execution details.). This tutorial will be of the greatest benefit if used while actually executing the program.

Compile and execute LASCAT application program.

****** PROGRAM LASCAT *******

The purpose of this program is to calculate the gas concentration and temperature profiles of a monolith catalyst section of a CO2 laser. The CO2 decomposes when the laser is pulsed. The CO and O2 produced as a result of pulsing are detrimental to the efficient operation of the laser. The recombination reaction is CO + 1/2 O2 -> CO. This program provides the means to model the performance of a monolith catalyst section under various gas compositions, temperatures, catalyst activities, gas flowrates, oxygen conversion, monolith face and length dimensions. Results can indicate if constraints such as conversion, maximum gas temperature, monolith weight are satisfied and how the system parameters may be altered to meet these constraints. Parameters and options may be altered to taylor the monolith design. Default values can also be used as a starting point for the design process. A review of the parameters and options chosen may be made prior to execution of the computational portion of the program.

(HIT RETURN TO CONTINUE)

A program introductory statement is presented. **Type RETURN** (key) after reading.

LASCAT Main Menu

1) Read in new operating parameters
2) Show current operating parameters
3) Change operating parameters
4) Run program
5) Exit program

Type in number corresponding to choice above.

The LASCAT Main Menu is presented. The main menu provides different options (1-5). Specific details for each option are provided in the Menu Description section. To choose one of these options, simply type in the desired number, then RETURN. For this example, **type 2 and RETURN.**

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00

Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): O2 conversion. %: 2.500
Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

The selectable parameter summary lists the parameter values that will be used in the computation portion of the program. When the program is initially run, default parameter values are assigned. As we'll see later, the values of the parameters can be changed. Hopefully, a review of the parameter summary above will hint to the meaning of each parameter. The use of each parameter is detailed in the Menu Description section. Let's assume the present values are satisfactory and proceed. **Type RETURN.**

LASCAT Main Menu

1) Read in new operating parameters
2) Show current operating parameters
3) Change operating parameters
4) Run program
5) Exit program

Type in number corresponding to choice above.

We have returned to the main menu. To save space, the main menu will listing will be abbreviated as "LASCAT Main Menu....". To run the computational portion of the program using the current parameter set listed in the selectable parameter summary **type 4 and RETURN.** Note: the program will alert you that it has completed computations by beeping three times.

*****SEE FILE LDATA FOR RESULTS*****
Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 39.063
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540

```
  Effective Diffusivity(cm^2/s)=     .053407
 Step size(mm) =                     .555556

Distance    %Conver  O2gas  O2wall  O2center   Tgas      Twall     DPress
 (mm)                  <===(mMOL/L)===>        (Kelvin)  (Kelvin)  (kPa)
  0.000     0.0000   .4065   .4060   .4058    300.000   300.179  -0.000E+00
  5.000     0.2239   .4052   .4048   .4046    300.236   300.416  -0.730E-05
 10.000     0.4574   .4040   .4035   .4033    300.474   300.656  -0.146E-04
 15.000     0.6933   .4027   .4022   .4020    300.714   300.897  -0.219E-04
 20.000     0.9314   .4014   .4009   .4008    300.956   301.141  -0.293E-04
 25.000     1.1718   .4001   .3996   .3994    301.201   301.388  -0.366E-04
 30.000     1.4146   .3988   .3983   .3981    301.448   301.637  -0.440E-04
 35.000     1.6598   .3975   .3970   .3968    301.697   301.888  -0.513E-04
 40.000     1.9075   .3961   .3957   .3955    301.949   302.141  -0.587E-04
 45.000     2.1577   .3948   .3943   .3941    302.204   302.398  -0.661E-04
 50.000     2.4104   .3934   .3930   .3928    302.461   302.656  -0.735E-04
 52.778     2.5519   .3927   .3922   .3920    302.605   302.801  -0.776E-04

Final values
 Mole fractions:
   He =  .2001 Ar = 0.0000 CO2 =  .3706
   CO =  .0195 O2 =  .0098 N2 =  .4001
 Gas Pressure (kPa):              101.325
 Reynolds number =                  9.817
 Gas Heat Capacity (J/K-g) =        1.799
 Gas Density (g/cm^3) =             .0011720
 Gas Velocity (mm/s) =             39.378
 Effectivness factor =              .99965
  Bulk Gas Diffusivity(cm^2/s)=     .22832
  Effective Diffusivity(cm^2/s)=    .053988
 Step size(mm) =                    .555556
```

==> Hit Return to Return to Main Menu <==

The information above provides initial and final values of important parameters along with values of key parameters along the length of the monolith. The units for each parameter are specified. A few minutes spent in reviewing the trend of each parameter, either initial vs. final or along the length of the monolith, is well worth the time. For example, the gas heat capacity increases from 1.797 to 1.799 due to the change in gas composition and the change in gas temperature. The gas temperature rises from 300.000 to 302.605 due to the exothermic nature of the reaction $CO + 1/2O_2 \rightarrow CO_2$. **Type RETURN.**

LASCAT Main Menu....

To change the value of a parameter or parameters, **type 3 and RETURN.**

Parameter Modification Menu

1) Change monolith physical dimensions
2) Change inlet gas composition
3) Change inlet gas volumetric flow rate
4) Change inlet gas temperature
5) Change inlet gas pressure
6) Change catalyst activation energy

7) Change catalyst reaction rate constant
8) Change catalyst active layer density
9) Change macro/micro pore radius & void-fraction
10) Change thermal operation(Adiabatic/Isothermal)
11) Change output profile (Full/ Summary)
12) Change termination variable(Conversion/Length)
13) Change computation display interval

14) Show current operating parameters
15) Save current operating parameters
16) Run program
17) Return to main menu
18) Exit program

Type in number corresponding to choice above

You have entered the Parameter Modification Menu. The Parameter Modification Menu gives a number of options (1-18). The parameters are detailed in the Program Operations section. The Parameter Modification Menu will be abbreviated "Parameter Modification Menu....". Let's change the termination variable (option 12). **Type 12 and RETURN.**

Integration can be stopped by either specifying
an amount of O2 conversion (O), or by specifying
a monolith length (L).

Currently , integration will be stopped
by specifying an amount of O2 conversion (O).

Type the letter O or the letter L. Hit return.

The letter L is for program computation section termination on monolith length. The letter O is for termination on O_2 conversion and requires a conversion length specification. **Type L and RETURN.**

Current desired monolith length = 5.000 (mm)

Input desired monolith length (5 - 4000mm)

The current restriction on the desired monolith termination length is given. The restrictions presented must be followed. Attempts have been made to prevent out of bounds values from being input, however "nothing is perfect". **Try entering 2** (this shorter than the minimum 5mm). The program will force a proper input. **Type 100 and RETURN.**

Parameter Modification Menu....

Let's see what has been changed. **Type 14 and RETURN.**

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Change ==> Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN. To avoid changing from the default parameter values to frequently used values, a parameter set can be saved to a file. These files can be read from at a later time. **Type 15 and RETURN.**

Would you like to save the current operating

parameters to a New(N) or Existing(E) file?

Were creating a new file. **Type N and RETURN.**

What's the name of the NEW
parameter file to be opened?

Name this file CATONE (abbreviation for CATALYST-ONE). **Type CATONE and RETURN.**

Parameter Modification Menu....

Using the revised parameter set, run the computational portion of the program by **typing 16 and RETURN.**

*****SEE FILE LDATA FOR RESULTS*****
Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 39.063
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas	Twall	DPress
		<===(mMOL/L)===>			(Kelvin)	(Kelvin)	(kPa)
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00

5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
55.000	2.6657	.3921	.3916	.3914	302.720	302.918	-0.809E-04
60.000	2.9236	.3907	.3902	.3900	302.983	303.182	-0.883E-04
65.000	3.1842	.3893	.3888	.3886	303.247	303.449	-0.957E-04
70.000	3.4475	.3879	.3874	.3872	303.515	303.718	-0.103E-03
75.000	3.7136	.3865	.3860	.3858	303.785	303.990	-0.111E-03
80.000	3.9825	.3851	.3846	.3843	304.058	304.265	-0.118E-03
85.000	4.2543	.3836	.3831	.3829	304.334	304.543	-0.126E-03
90.000	4.5290	.3822	.3817	.3814	304.613	304.824	-0.133E-03
95.000	4.8066	.3807	.3802	.3800	304.895	305.108	-0.141E-03
100.000	5.0873	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values
Mole fractions:
He = .2001 Ar = 0.0000 CO2 = .3712
CO = .0190 O2 = .0095 N2 = .4002
Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm^3) = .0011624
Gas Velocity (mm/s) = 39.693
Effectivness factor = .99961
Bulk Gas Diffusivity(cm^2/s)= .23125
Effective Diffusivity(cm^2/s)= .054566
Step size(mm) = .555556

==> Hit Return when finished viewing <==

In addition to the screen output the selectable parameter summary and the section above are written to file LDATA(Macintosh) or LDATA.DAT(VAX). (For Macintosh only: Any additional "runs" in this session will be tacked on to the end of LDATA. If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in LDATA, rename LDATA prior to running LASCAT again.) **Type RETURN.**

LASCAT Main Menu....

After each computational run, you are returned to the main menu. Let's change another parameter. **Type 3 and RETURN.**

Parameter Modification Menu....

To change the inlet gas volumetric flow rate, **type 3 and RETURN.**

Current inlet volumetric
flow rate = .250 (l/s)

Input monolith inlet volumetric flow rate

The desired flowrate is 2.5 liters/sec. **Type 2.5 and RETURN.**

Parameter Modification Menu....

Let's examine the change to the parameter set. **Type 14 and RETURN.**

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Change ==> Gas Flow rate(liters/s): 2.500 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): 5.0000 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN.

Parameter Modification Menu....

Run computational portion of the program by **typing 16 and RETURN**

*****SEE FILE LDATA FOR RESULTS*****
Initial values
Reynolds number = 98.802
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 390.625
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = 5.000000

Distance	%Conver	O2gas	O2wall	O2center	Tgas	Twall	DPress

(mm)		<===(mMOL/L)===>			(Kelvin)	(Kelvin)	(kPa)
.000	.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	.0156	.4064	.4059	.4057	300.024	300.203	-0.730E-04
10.000	.0391	.4062	.4058	.4056	300.047	300.227	-0.146E-03
15.000	.0624	.4061	.4057	.4055	300.071	300.250	-0.219E-03
20.000	.0855	.4060	.4055	.4054	300.095	300.274	-0.292E-03
25.000	.1086	.4059	.4054	.4052	300.119	300.298	-0.365E-03
30.000	.1317	.4057	.4053	.4051	300.142	300.322	-0.438E-03
35.000	.1549	.4056	.4052	.4050	300.166	300.346	-0.511E-03
40.000	.1781	.4055	.4050	.4049	300.190	300.370	-0.584E-03
45.000	.2013	.4054	.4049	.4047	300.214	300.394	-0.657E-03
50.000	.2245	.4052	.4048	.4046	300.238	300.418	-0.730E-03
55.000	.2478	.4051	.4047	.4045	300.261	300.442	-0.803E-03
60.000	.2711	.4050	.4045	.4043	300.285	300.466	-0.877E-03
65.000	.2944	.4049	.4044	.4042	300.309	300.490	-0.950E-03
70.000	.3177	.4047	.4043	.4041	300.333	300.514	-0.102E-02
75.000	.3411	.4046	.4041	.4040	300.357	300.538	-0.110E-02
80.000	.3644	.4045	.4040	.4038	300.381	300.562	-0.117E-02
85.000	.3879	.4043	.4039	.4037	300.405	300.587	-0.124E-02
90.000	.4113	.4042	.4038	.4036	300.429	300.611	-0.132E-02
95.000	.4347	.4041	.4036	.4034	300.453	300.635	-0.139E-02
100.000	.4582	.4040	.4035	.4033	300.477	300.659	-0.146E-02

==> Hit Return to Return to Main Menu <==

Notice that the program computation terminated when the monolith length reached 100 mm, whereas, previously, the termination condition was an oxygen conversion of 2.5 %. **Type RETURN.**

LASCAT Main Menu....

The parameter set has been changed from the CATONE set. Let's return to the CATONE parameter set by reading in the CATONE set file. **Type 1 and RETURN.**

Read in data from existing parameter file?(Y/N)

Type Y and RETURN.

What is the name of the existing parameter file to be opened?

Type CATONE and RETURN (Note that the required file name to be inputted may be lower /upper case sensitive).

LASCAT Main Menu....

Let's review the parameter set. **Type 2 and RETURN.**

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000

Change ==> Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN.

LASCAT Main Menu....

Let's explore the use of some other parameters. **Type 3 and RETURN.**

Parameter Modification Menu....

Type 11 and RETURN.

Full concentration and temperature profile (P) or summary (S)?
Type the letter P or the letter S. HIT RETURN.

Choose summary by **typing S and RETURN.**

Parameter Modification Menu....

Type 16 and RETURN.

*****SEE FILE LDATA FOR RESULTS*****
Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 39.063
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = .555600

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
		<===(mMOL/L)===>					
.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
100.008	5.0878	.3792	.3787	.3785	305.180	305.395	-0.148E-03

```
Final values
 Mole fractions:
   He =  .2001 Ar = 0.0000 CO2 =  .3712
   CO =  .0190 O2 =  .0095 N2 =  .4002
 Gas Pressure (kPa):              101.325
 Reynolds number =                  9.753
 Gas Heat Capacity (J/K-g) =        1.800
 Gas Density (g/cm^3) =              .0011624
 Gas Velocity (mm/s) =             39.693
 Effectivness factor =               .99961
  Bulk Gas Diffusivity(cm^2/s)=      .23125
  Effective Diffusivity(cm^2/s)=     .054566
 Step size(mm) =                     .555600

          ==> Hit Return to Return to Main Menu <==
```

The key parameters along the length of the monolith are presented for the initial and final (termination condition met) monolth distances. The file LDATA also has this summary form. **Type RETURN.**

```
                    LASCAT Main Menu....
```

Please feel free to play around with the program. To exit the program by **type 5 and RETURN. Take a look at files, LDATA and CATONE.** A listing of both files is given below. The table entries are separated by tab characters for further processing by programs such as Cricket Graph and Excel (these are both Macintosh programs). Adjusting the tabs to 1 space may help to align the table.

File LDATA

```
                SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness:  1.00   Face dimension:  100.00 x  100.00
Channel inner dimension:  4.00   No.Face channels:  20.00   x  20.00
Active layer thickness:  .25    % monol.volume open :  64.0
Monolith inlet parameters:
Gas Composition (mole fraction):   CO2:  .3700  CO:  .0200  O2:  .0100
                                   N2:  .4000  He:  .2000  Ar: 0.0000
Gas Flowrate(liters/s):   .250  Gas Temperature(K):  300.00
Inlet Gas Pressure (kPa):  101.325
Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s):   123.40
Activation energy(J/mol):   39700.00
Void-fraction as micropores:  .24   Void-fraction as macropores:  .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): O2 conversion.  %:   2.500
Computation loop step size(mm):  .5556   Display every  5.00 mm

Initial values
 Reynolds number =                  9.880
 Gas Heat Capacity (J/K-g) =        1.797
 Gas Density (g/cm^3) =              .0011817
 Gas Velocity (mm/s) =             39.063
 Effectivness factor =               .99969
  Bulk Gas Diffusivity(cm^2/s)=      .22540
```

Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas	Twall	DPress
		<===(mMOL/L)===>			(Kelvin)	(Kelvin)	(kPa)
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
52.778	2.5519	.3927	.3922	.3920	302.605	302.801	-0.776E-04

Final values
Mole fractions:
He = .2001 Ar = 0.0000 CO2 = .3706
CO = .0195 O2 = .0098 N2 = .4001
Gas Pressure (kPa): 101.325
Reynolds number = 9.817
Gas Heat Capacity (J/K-g) = 1.799
Gas Density (g/cm^3) = .0011720
Gas Velocity (mm/s) = 39.378
Effectivness factor = .99965
Bulk Gas Diffusivity(cm^2/s)= .22832
Effective Diffusivity(cm^2/s)= .053988
Step size(mm) = .555556

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0
Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325
Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): .5556 Display every 5.00 mm

Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 39.063
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
		<===(mMOL/L)===>					
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
55.000	2.6657	.3921	.3916	.3914	302.720	302.918	-0.809E-04
60.000	2.9236	.3907	.3902	.3900	302.983	303.182	-0.883E-04
65.000	3.1842	.3893	.3888	.3886	303.247	303.449	-0.957E-04
70.000	3.4475	.3879	.3874	.3872	303.515	303.718	-0.103E-03
75.000	3.7136	.3865	.3860	.3858	303.785	303.990	-0.111E-03
80.000	3.9825	.3851	.3846	.3843	304.058	304.265	-0.118E-03
85.000	4.2543	.3836	.3831	.3829	304.334	304.543	-0.126E-03
90.000	4.5290	.3822	.3817	.3814	304.613	304.824	-0.133E-03
95.000	4.8066	.3807	.3802	.3800	304.895	305.108	-0.141E-03
100.000	5.0873	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values
Mole fractions:
He = .2001 Ar = 0.0000 CO2 = .3712
CO = .0190 O2 = .0095 N2 = .4002
Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm^3) = .0011624
Gas Velocity (mm/s) = 39.693
Effectivness factor = .99961
Bulk Gas Diffusivity(cm^2/s)= .23125
Effective Diffusivity(cm^2/s)= .054566
Step size(mm) = .555556

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0
Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flowrate(liters/s): 2.500 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325
Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): 5.0000 Display every 5.00 mm

Initial values
Reynolds number = 98.802
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817

Gas Velocity (mm/s) = 390.625
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = 5.000000

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
		<===(mMOL/L)===>					
0.000	.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	.0156	.4064	.4059	.4057	300.024	300.203	-0.730E-04
10.000	.0391	.4062	.4058	.4056	300.047	300.227	-0.146E-03
15.000	.0624	.4061	.4057	.4055	300.071	300.250	-0.219E-03
20.000	.0855	.4060	.4055	.4054	300.095	300.274	-0.292E-03
25.000	.1086	.4059	.4054	.4052	300.119	300.298	-0.365E-03
30.000	.1317	.4057	.4053	.4051	300.142	300.322	-0.438E-03
35.000	.1549	.4056	.4052	.4050	300.166	300.346	-0.511E-03
40.000	.1781	.4055	.4050	.4049	300.190	300.370	-0.584E-03
45.000	.2013	.4054	.4049	.4047	300.214	300.394	-0.657E-03
50.000	.2245	.4052	.4048	.4046	300.238	300.418	-0.730E-03
55.000	.2478	.4051	.4047	.4045	300.261	300.442	-0.803E-03
60.000	.2711	.4050	.4045	.4043	300.285	300.466	-0.877E-03
65.000	.2944	.4049	.4044	.4042	300.309	300.490	-0.950E-03
70.000	.3177	.4047	.4043	.4041	300.333	300.514	-0.102E-02
75.000	.3411	.4046	.4041	.4040	300.357	300.538	-0.110E-02
80.000	.3644	.4045	.4040	.4038	300.381	300.562	-0.117E-02
85.000	.3879	.4043	.4039	.4037	300.405	300.587	-0.124E-02
90.000	.4113	.4042	.4038	.4036	300.429	300.611	-0.132E-02
95.000	.4347	.4041	.4036	.4034	300.453	300.635	-0.139E-02
100.000	.4582	.4040	.4035	.4033	300.477	300.659	-0.146E-02

Final values
Mole fractions:
He = .2000 Ar = 0.0000 CO2 = .3701
CO = .0199 O2 = .0100 N2 = .4000
Gas Pressure (kPa): 101.324
Reynolds number = 98.705
Gas Heat Capacity (J/K-g) = 1.798
Gas Density (g/cm^3) = .0011800
Gas Velocity (mm/s) = 391.188
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22592
Effective Diffusivity(cm^2/s)= .053513
Step size(mm) = 5.000000

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0
Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325
Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
Output file (Full Profile/Summary): Summary
Termination on (O2 conversion/Length): Length. Length(mm): 100.000

```
 Computation loop step size(mm):   .5556

Initial values
  Reynolds number =                 9.880
   Gas Heat Capacity (J/K-g) =      1.797
   Gas Density (g/cm^3) =            .0011817
   Gas Velocity (mm/s) =           39.063
   Effectivness factor =              .99969
    Bulk Gas Diffusivity(cm^2/s)=   .22540
    Effective Diffusivity(cm^2/s)=  .053407
   Step size(mm) =                   .555600

 Distance    %Conver  O2gas  O2wall  O2center     Tgas      Twall      DPress
  (mm)                 <===(mMOL/L)===>          (Kelvin)  (Kelvin)    (kPa)
   0 .000    0.0000    .4065   .4060    .4058   300.000    300.179  -0.000E+00
 100.008     5.0878    .3792   .3787    .3785   305.180    305.395  -0.148E-03

 Final values
   Mole fractions:
     He =  .2001 Ar = 0.0000 CO2 =  .3712
     CO =  .0190 O2 =  .0095 N2 =  .4002
   Gas Pressure (kPa):           101.325
   Reynolds number =               9.753
   Gas Heat Capacity (J/K-g) =     1.800
   Gas Density (g/cm^3) =           .0011624
   Gas Velocity (mm/s) =          39.693
   Effectivness factor =              .99961
    Bulk Gas Diffusivity(cm^2/s)=  .23125
    Effective Diffusivity(cm^2/s)= .054566
   Step size(mm) =                  .555600
```

File CATONE. See if you can pick out some of the parameters listed below. The program listing will show the structure of the parameter file.

```
 100.0
 100.0
 .5000
 4.000
 4.000
 .2500
 .2000
 1.0000E-07
 .3700
 2.0000E-02
 1.0000E-02
 .4000
 1.000
A
P
L
 2.500
 100.0
 3.9700E+04
 123.4
 300.0
 .2500
9
 .5556
 5.0000E-04
 .2400
 .4800
 12.00
 500.0
```

Appendix 3: Menu Description

LASCAT Main Menu

The LASCAT Main Menu section provides detailed instructions on the use of the main menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT Main Menu is first encountered upon program execution and has five options available. Each option is detailed below. To select an option type the desired choice (1- 5) and then RETURN (key). A number other than 1-5 will cause an input requirement message to appear and another chance to enter 1-5 is made available.

Option 1 - Read in new operating parameters:

If you have a file containing a selectable parameter set that you want to use, choose this option. This file would have been previously generated by saving the parameter set using option 15 of the parameter modification menu. You will first be queried whether the file is New (N) or Existing (E). the file is Existing (E). If you indicate that the file is existing, you will be queried for the file name. Some systems are sensitive to upper and lowercase differences in file names. After specifying the filename, you are returned to the main menu. If you indicate that the file is new, default file parameters are assigned.

Option 2 - Show current operating parameters:

This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the main menu.

Option 3 - Change operating parameters:

This option leads to the parameter modification menu described below. The options similar to main menu options 1-5 are available in the parameter modification menu. You can return to the main menu from the parameter modification menu.

Option 4 - Run program:

The Run program option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in the session will be tacked on to the end of file LDATA. (Macintosh only: If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu.

Option 5 - Exit program:

The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above in the Option 4 section.

LASCAT Parameter Modification Menu

The LASCAT parameter modification menu section provides detailed instructions on the use of the parameter modification menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT parameter modification menu is encountered when option 3 of the main menu is chosen and has eighteen options available. Each option is detailed below. To select an option type the desired choice (1-18) and then RETURN. A number other than 1-18 will cause an input requirement message to appear and another chance to enter 1-18 is made available. The default file parameter set is the parameter set is instituted at the start of the program.

Option 1 - Change monolith physical dimensions:

A number of physical dimensions (see diagram below) are queried for in this section. A description of each dimension and the associated restrictions are listed. Values that represent a valid physical situation and meet the listed restrictions should not cause any problems. A number of constraint for given below. The program assumes monolith channels are square. Remember that the system under study can be scaled up or down. For instance, a monolith with an inlet gas flow rate of 1 liters/sec and a face (H x V) of 100 x100 mm can be scaled up to an inlet gas flow rate of 4 liters/sec and a face of 200 x 200mm. The other dimensions (H,W, and A) are held the same.

Monolith horizontal face dimension (mm), H, $10 \leq H \leq 1000$
Monolith vertical face dimension (mm), V, $10 \leq V \leq 1000$
Monolith channel wall thickness (mm), T, $T \leq H$, $T \leq V$
Monolith channel opening dimension (mm) , W, $W \leq H$, $W \leq V$
Monolith active layer thickness (mm) , A , $A \leq W/2$
Default file dimension values(mm) are H=V=100.0, T=0.50, W=4.00, and A=0.25

Monoliths with square channels but with circular, oval, etc., shaped faces can be modelled. For these nonstandard shapes, determine the dimensions (H x V) of a square faced monolith that has an equivalent facial area and use the calculated H and V in the program.

Option 2 - Change inlet gas composition:

The program allows for the laser operating gas to contain He, Ar, CO_2, O_2, CO, and N_2 gases. The species mole fraction is defined as the mole percent divided by 100. For example, 10 mole% N_2 corresponds to a mole fraction of 0.10. Each mole fraction must be between 0 and 1. Mole fractions for He, Ar, CO_2, O_2 are quieried for when this option is chosen. Stoichiometric ratios of O_2:CO (1:2) are assumed; the input mole fraction of O_2 is used to calculate the CO mole fraction. The mole fraction of O_2 is limited to 0.03 (3%).The sum of the mole fractions must add up to 1; N_2 mole fraction is calculated using the mole fractions of the other species. The default file values for mole fractions are He=0.20, Ar=0.0, CO_2=0.37, O_2=0.01, CO=0.02, and N_2=0.40.

Option 3 - Change inlet gas volumetric flow rate:

Inlet gas volumetric flow rate (liters/sec) is queried for in this option. The inlet flow rate is assumed to be at the temperature specified in option 4. Although there is no upper limit on the inlet gas flow rate, if the flow rate results in a Reynolds (Re) number > 2300, the computational portion of the program will be terminated. The default file value is 0.25 liters/sec.

Option 4 - Change inlet gas temperature:

Inlet gas temperature (K) is quieried for in this option. The acceptable range of temperature is 200 to 700 K. Gas temperature is updated along the length of the monolith. If the gas temperature reaches 700 K along the length of the monolith the computational portion of the program will be terminated. The default file inlet gas temperature is 300 K.

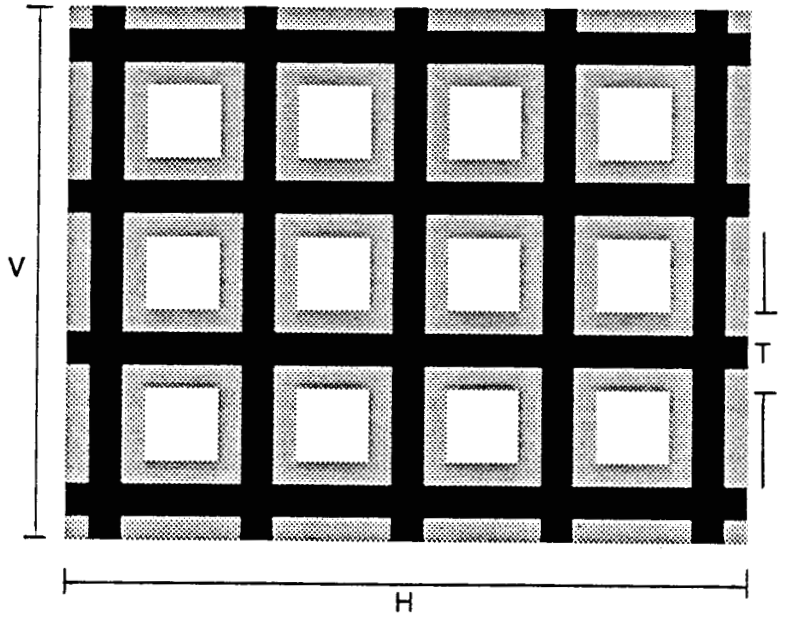
Option 5 - Change inlet gas pressure:

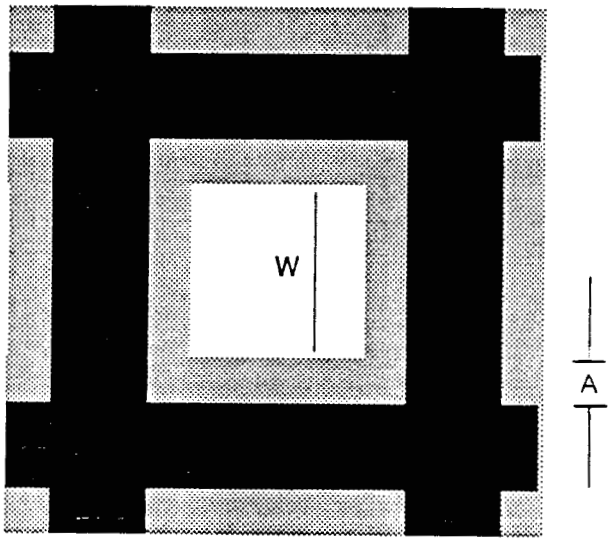
Inlet gas pressure (kPa) is quieried for in this option. The acceptable range for inlet gas pressure is 0.1 to 350 kPa. The pressure is updated along the length of the monolith. If the gas pressure exceeds 350 kPa or drops below 0.1kPa along the length of the monolith the computational portion of the program will be terminated. The default file value is 101.325 kPa (1atm).

Option 6 - Change catalyst activation energy:

Catalyst activation energy (J/mol) is quieried for in this option. The acceptable range for catalyst activation energy is between 0 and 300,000 J/mol. The default file value is 39700 J/mol.

Option 7 - Change catalyst reaction rate constant:





Catalyst reaction rate constant (mm^3/gcat-sec) [referenced to 298 K] is quieried for. The catalyst activation energy must be greater than zero. The default file value is 123.4 mm^3/gcat-sec.

Option 8 - Change catalyst active layer density:

Catalyst active layer density (g/mm^3) is quieried for in this option. The catalyst active layer density must be greater than zero. The default file value is 5e-04 g/mm^3.

Option 9 - Change macro/micro pore radius & void-fraction:

Four quantities, macropore and micropore radius and macropore and micropore void-fractions, are queried for in this option.
Define macropore radius (nm) = RMACRO Default value= 500 nm
Define micropore radius (nm) = RMICRO Default value= 12 nm
Define macropore void-fraction = EMACRO Default value= 0.48
Define micropore void-fraction = EMICRO Default value= 0.24
Acceptable ranges: RMICRO < RMACRO, EMACRO + EMICRO ≤ 1.0

Option 10 - Change thermal operation (Adiabatic/Isothermal):

Type of monolith thermal operation (adiabatic/isothermal) is quieried for in this option. For isothermal operation the gas and the monolith section are maintained at (or very close to)the gas inlet temperature specified in option 4. Default file operation mode is adiabatic.

Option 11 - Change output profile (Full/ Summary):

Type of output profile is quieried for in this option. Only the initial and final values (temperature, pressure, and O_2 concentration) are output in the summary option. In the full option, the values are specified for each display interval as specified in option 13. Default file value is Full. See LASCAT Tutorial for an example.

Option 12 - Change termination variable (Conversion/Length):

The termination condition (O_2 conversion or monolith length) is queried for in this option. If O_2 conversion is chosen, the termination percent conversion (0-100 %) is required to be specified The default O_2 conversion is 2.5 % If the monolith length option is chosen, the monolith length (5-4000mm) is required to be specified. The default monolith length is 5mm. See LASCAT Tutorial for an example.

Option 13 - Change computation display interval:

Computaion display interval (CDI) is quieried for in this option. The display interval specifies the reporting interval for temperature, pressure, and O_2 concentration. The specified display interval may be over overriden if too many computational loop iterations (>250) are required to meet the specified display interval. The default file value is 5mm.

Option 14 - Show current operating parameters:

This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the parameter modification menu. This option is similar to option 2 of the main menu.

Option 15 - Save current operating parameters:

This option allows the user to save the current operating parameter set to file. The file name and the file status (new or existing) are required to be specified. The main menu's option 1 allows parameter set files to be installed as the current selectable parameter set.

Option 16 - Run program:

The "Run program" option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in this session will be tacked on to the end of file LDATA. (Macintosh only: If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu. This option is identical to option 4 of the main menu.

Option 17 - Return to main menu:

Returns to the main menu. See main menu seciton above.

Option 18 - Exit program:

The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above.

```
C************************PROGRAM LASCAT************************
C Written by
C  Keith Guinn, Seth Goldblum Dr. Richard Herz,and Ed Noskowski
C  Department of AMES / Chemical Engineering  B-010
C  University of California, San Diego
C  La Jolla, CA 92093
C
C Date revised-February 1989
C
C Funded by NASA's Langley Research Center GRANT  No. NAG-1-823
C
C Fortran Software Compatibility
C  MICROSOFT FORTRAN Version 2.2 (MACINTOSH PLUS,SE, & II)
C  ABSOFT MacFORTRAN/020 Version 2.3 (MACINTOSH II)
C  This program is FORTRAN 77 compatible.
C
C Editing program used: QUED Version 1.53 (MACINTOSH)
C
C Program listing outline                                line numbers
C   1. Program information and table of contents          2 -35
C   1. Indentifiers                                      36 -153
C   2. Program Algorithm/Restrictions                   154 -297
C   3. Program LASCAT                                   298 -1450
C     A. Variable declaration                           299 -322
C     B. Introduction/purpose                           323 -357
C     C. Default/read/write parameters                  358 -457
C     D. Main-menu, Sub-menu                            457 -551
C     E. Parameter input section, write parameters      552 -981
C     F. Initialize physical properties                 982 -1038
C     G. Step size check loop                          1039 -1116
C     H. Main computational loop                       1162 -1409
C   4. Subroutines: RK4,FUNC,LINES,HEADER              1451 -1906
C                   TCON,PROP,VIS,FXN1
C                   FXN2,FXN3,FXN4
C
C*********************    IDENTIFIERS   *********************************
C A-REACTION RATE CONSTANT OF ACTIVE CATALYST MATERIAL (mm^3/g-cat s)
C AMW-AVERAGE MOLECULAR WEIGHT OF GAS MIXTURE (g/mole)
C AREF-VOLUMETRIC PUMPING RATE OF ACTIVE CATALYST AT 298K(mm^3/g-cat s)
C ASK-QUERY DIRECTION NUMBER
C AX(i,j)-i,j=1->6** CROSS TERM MATRIX FOR THERMAL CONDUCTIVITY
C BEEP-BEEP CHARACTER
C CDI=COMPUTATION DISPLAY INTERVAL(mm)
C CGX-MONOLITH CHANNEL O2 GAS CONC. AT POSITION X (mol/mm^3)
C CGXTMP-MONOLITH CHAN. O2 GAS CONC. AT POSITION X-DX (mol/mm^3)
C     THIS IS A HOLDING CONSTANT TO DETERMINE DCGX
C CGXZ-MONOLITH CHAN. O2 GAS CONC. AT POSITION X=0 (mol/mm^3)
C CH,CH1,CH2 - CHARACTER*1 Dummy Variable
C CHFLO-MONOLITH CHANNEL VOLUMETRIC FLOWRATE (mm^3/s)
C CHGVEL-MONOLITH CHANNEL GAS VELOCITY (mm/s)
C CHHD-MONOLITH CHANNEL HYDRAULIC DIAMETER (mm)
C CHSTV-MONOLITH CHANNEL SURFACE AREA TO VOLUME (1/mm)
C CHWP-MONOLITH CHANNEL WETTED PERIMETER (mm)
C CMCWT-CHARACTERISTIC MCWT(mm)
C CONST1,CONST2,CONST3,CONST4,CONST5-RESULT HOLDING CONSTANTS
C CONST5,CONST6,CONST7,CONST8,CONST9-RESULT HOLDING CONSTANTS
C CONSTA,CONSTB,CONSTD,CONSTE,CONSTF,CONSTC-RESULT HOLDING CONSTS
```

```
C CONV-CONVERSION OF OXYGEN IN MONOLITH CHANNEL (%)
C CONVX-CONVERSION OF OXYGEN AS FUNCTION OF X (%)
C CONVXZ-CONVERSION OF OXYGEN AT X=0 (%)
C CP(i),i=1,6-HEAT CAPACITY OF SPECIES i AT TEMP. TGX (J/K-g)
C CPGAS-HEAT CAPACITY OF BULK GAS MIXTURE (J/K-g)
C CPCAT-HEAT CAPACITY OF CATALYST WASHCOAT (J/K-g)
C CPSUP-HEAT CAPACITY OF MONOLITH SUPPORT (J/K-g)
C CSX-MONOLITH CHAN. WALL O2 GAS CONC AT POSIT. X (mol/mm^3)
C CSXZ-MONOLITH CHAN. WALL O2 GAS CONC AT POSIT X=0 (mol/mm^3)
C D(i),i=1-6-BINARY DIFF COEFF FOR O2 in i 298K,1atm (mm^2/s) C
C DAB-DIFFUSIVITY OF O2 IN BULK GAS (mm^2/s)
C DABEFF-EFFECTIVE DIFFUSIVITY OF O2 IN WASHCOAT (mm^2/s)
C DCGX-CHANGE IN CGX FOR A CHANGE DX(mol/mm^3)
C DENGAS-DENSITY OF BULK GAS MIXTURE (g/mm^3)
C DENGSR-REFERENCE DENSITY OF BULK GAS MIXTURE (g/mm^3)
C DENCAT-DENSITY OF CATALYST WASHCOAT (g/mm^3)
C DENSUP-DENSITY OF MONOLITH SUPPORT (g/mm^3)
C DP-PRESS CHANGE ASSOC. WITH A CHANGE IN CHANNEL POSITION DX(atm)
C DFGX- CHANGE IN FGX FOR A CHANGE  DX (MOL/s)
C DKMICR-KNUDSEN DIFFUSION COEFFICIENT IN MICROPORES (mm^2/s)
C DKMACR-KNUDSEN DIFFUSION COEFFICIENT IN MACROPORES (mm^2/s)
C DMICRO-EFFECTIVE DIFFUSION COEFFICIENT IN MICROPORES (mm^2/s)
C DMACRO-EFFECTIVE DIFFUSION COEFFICIENT IN MACROPORES (mm^2/s)
C DTGX-CHANGE IN TGX FOR A CHANGE DX(mol/mm^3)
C DX-INCREMENTAL CHANGE IN MONOLITH CHANNEL POSITION X (mm)
C DXCHK-COUNTS # OF TIMES THROUGH THE LOOP DURING STEP SIZE CHECK
C EMICRO-FRACTION OF TOTAL VOIDS IN PELLETS AS MICROPORES
C EMACRO-FRACTION OF TOTAL VOIDS IN PELLETS AS MACROPORES
C ENGACT-CATALYST REACTION ACTIVATION ENERGY(J/mol)
C FZERO - INLET 02 MOLAR FLOWRATE (MOL/s)
C FACTOR-PROFILE STEP SIZE FACTOR (integer)
C FGX - MOLAR FLOWRATE OF O2 AT POSITION X (MOL/s)
C FGXEND - OUTLET O2 MOLAR FLOWRATE (MOL/s)
C FILNAM - NAME OF DATAFILE CONTAINING DEFAULT PARAMETERS
C FIRST - LOGICAL*1 IS TRUE IF FIRST TIME THROUGH LOOP, AND
C     FALSE IF ANYTHING ELSE
C H-HEAT TRANSFER COEFFICIENT FROM GAS TO WALL (J/mm^2-s-K)
C HEATRX- NEGATIVE CHANGE IN ENTHALPY FOR 02+2CO->CO2 REACTION(J/mol)
C I,J-INTEGER COUNTER
C JUMP-INTEGER- VALUE DETERMINES IF DX CAN BE FURTHER REDUCED
C K-THERMAL GAS CONDUCTIVITY (J/mm-s-K)
C KC-MASS TRANSFER COEFFICIENT(mm/s)
C KREF-REFERENCE THERMAL GAS CONDUCTIVITY (J/mm^2-s-K)
C LAMBMX - THERMAL CONDUCTICITY OF THE BULK GAS MIXTURE (mW/cm K)
C MAIN - BOOLEAN EXPRESSION. TRUE WHEN USER IS IN MAIN MENU
C MCH-MONOLITH CHANNEL HEIGHT (mm)
C MCST-MONOLITH CHANNEL SUPPORT WALL THICKNESS (mm)
C MCW-MONOLITH CHANNEL WIDTH (mm)
C MCWT-MONOLITH CHANNEL WASHCOAT THICKNESS (mm)
C MFDH-MONOLITH HORIZONTAL FACE DIMENSION(mm)
C MFDV-MONOLITH VERTICAL FACE DIMENSION(mm)
C MOLFLO - MOLAR FLOWRATE OF BULK GAS THROUGH MONOLITH (M/s)
C MONOL-COMPUTATION LOOP COMPLETION MONOLITH LENGTH(mm)
C MVFLO-MONOLITH VOLUMETRIC GAS FLOWRATE(mm^3/s)
C MVFLZ-INLET MONOLITH VOLUMETRIC GAS FLOWRATE(mm^3/s)
C MW(i)-i->1,6** MOLECULAR WEIGHT OF COMPONENT GASES(gms/mole)
C N-EFFECTIVESS FACTOR FOR CATALYST WASHCOAL (NONDIM)
```

```
115 C NOCHM-NUMBER OF CHANNELS IN MONOLITH
116 C NOCHV-NUMBER OF CHANNELS VERTICALLY IN MONOLITH
117 C NOCHH-NUMBER OF CHANNELS HORIZONTALLY IN MONOLITH
118 C O2ZERO-MONOLITH INLET OXYGEN CONCENTRATION (%O2)
119 C ONCE-INTEGER-DETERMINES IS THIELE STATEMENT HAS BEEN WRITTEN
120 C P-DO LOOP VARIABLE
121 C PZERO-INLET PRESSURE OF GAS MIXTURE (atm)
122 C PRESS-PRESSURE OF GAS MIXTURE IN THE CHANNEL(atm)
123 C Q-HOLDING CONSTANT
124 C R-GAS CONSTANT  (J/mol-K)
125 C RE - Reynold's number (dimensionless)
126 C RMICRO-AVERAGE MICROPORE RADIUS (cm)
127 C RMACRO-AVERAGE MACROPORE RADIUS (cm)
128 C S-TAB CHARACTER
129 C SS-CARRIAGE RETURM CHARACTER
130 C SSS-A OR I FOR ADIABATIC OR ISOTHERMAL-CHARACTER
131 C SSS1-P OR S FOR PROFILE OR SUMMARY-CHARACTER
132 C SSS2-O OR L FOR O2 CONVERSION OR MONOLITH LENGTH-CHARACTER
133 C T-GAS TEMPERATURE FOR VISCOSITY AND THERMAL CONDUCTIVITY
134 C TCON(i,j)-i->1,6**,j->2,7***,THERMAL COND. OF COMPONENT GASES
135 C     AT VARIOUS TEMPERATURES(mW/cm-K)
136 C TCONT(i)-i->1,6**THERM COND.OF COMPONENT GASES,@TEMP T (mW/cm*K)
137 C TGX-MONOLITH CHANNEL BULK GAS TEMPERATURE AT POSIT. X (K)
138 C THIELE-SLAB THIELE MODULUS FOR CATALYST WASHCOAT (NONDIM)
139 C TREF-PHYSICAL PROPERTIES REF TEMP=298K (K)
140 C TSX-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X (K)
141 C TSXZ-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X=0 (K)
142 C TZERO-MONOLITH INLET GAS TEMPERATURE (K)
143 C VISC(i,j)-i->1,6**,j->2,7***,VISCOSITY OF COMPONENT GASES
144 C     AT VARIOUS TEMPERATURES(centipoises)
145 C VISCT(i)-i->1,6** VISCOS OF COMP GASES @ TEMP T(centipoises)
146 C VISCTC-COMPOSITE GAS VISCOSITY(centipoises)
147 C X-MONOLITH CHANNEL POSITION (mm)
148 C XZ-MONOLITH CHANNEL POSITION AT X=0 (mm)
149 C Y(i)-i->1,6** MOLE FRACTION OF COMPONENT GASES(gms/mole)
150 C Y10,Y20,Y30,Y40,Y50,Y60-HOLDING CONSTANTS FOR Y(i)'s
151 C  **1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2
152 C  ***2=200, 3=300, 4=400, 5=500, 6=600, 7=700K
153 C
154 C***********     PROGRAM ALGORITHM/RESTRICTIONS  *********************
155 C  -Declare variables
156 C  -Open output data file "LDATA" using unit 25
157 C  -Display introduction on screen
158 C  -Read in values of default operating parameters
159 C  -Compute some geometric and record starting values using default
160 C        parameters
161 C  -Display main menu, query for desired option (1-5)
162 C   1-Read in new operating parameters
163 C     -Query for file from which to read from
164 C     -Read in values from file
165 C     -Return to main menu
166 C   2-Show current operating parameters
167 C     -Display operating parameter summary table, this includes some
168 C      calculated values
169 C     -Return to main menu
170 C   3-Change operating parameters
171 C     -Drop to submenu, query for desired option (1-18), if not 1-18
```

```
172 C          query again.  After each section is completed return to
173 C          the submenu.
174 C       -1 Change monolith physical dimensions (mm)
175 C          -Input monolith face dimensions (vertical & horizontal)
176 C             range: >=10mm, <=1000mm
177 C          -Input monolith channel wall thickness, inner channel
178 C             dimension, active layer thickness
179 C             range: support wallthickness
180 C                       < either vert. or horiz face
181 C             range: inner channel dimension
182 C                       < either vert or horiz face
183 C             range: active layer thickness < 0.5 * ( support wall)
184 C          -Recompute some geometric parameters using new dimensions
185 C       -2 Change Inlet Gas Composition(mole fractions)
186 C          -Input mole fractions of He, Ar, CO2, and O2
187 C          -Mole fraction of CO is set to twice that of O2
188 C          -Mole fraction of N2 is computed to make mole fraction
189 C             sum equal to one
190 C             range:each mole fraction >=0 and <=1,
191 C             sum mole fractions =1
192 C       -3 Change inlet gas volumetric flowrate(l/s)
193 C          -Input inlet volumetric flowrate
194 C             range: volumetric flowrate >0
195 C       -4 Change inlet gas temperature(Kelvin)
196 C          -Input inlet gas temperature
197 C             range: temperature >=200K and <=700K
198 C       -5 Change inlet gas pressure(kPa)
199 C          -Input inlet gas pressure(kPa)
200 C             range: pressure 0.1-350 kPa
201 C       -6 Change catalyst activation energy(J/mol)
202 C          -Input caltalyst activation energy(J/mol)
203 C             range: activation energy >0 and <300000
204 C       -7 Change catalyst reaction rate constant(mm^3/gcat-s)
205 C          -Input reaction rate constant
206 C             range: reaction rate >0
207 C       -8 Change catalyst active layer density(g/mm^3)
208 C          -Input density
209 C             range: density >0
210 C       -9 Change macro/micro pore radius & void-fraction
211 C          -Input macro/micro pore radius
212 C              range: radius >0 , micro<macro
213 C          -Input macro/micro void-fractions
214 C              range: sum <=1 , void-fractions>=0
215 C       -10 Change thermal operation (Adiabatic/Isothermal)
216 C          -Input option A/I or a/i
217 C       -11 Change output profile (Full/ Summary)
218 C          -Input option P/S or p/s
219 C       -12 Change termination variable (Conversion/Length)
220 C          -Input termination option O2 conversion(O) or monolith
221 C              monolith lenght(L). If (O) is chosen, specific
222 C              termination conversion (%O2).  If (L) is chosen specify
223 C              monolith length(mm).  O2% conversion range >0,<100%.
224 C              Monolith length range >5, <4000mm.
225 C       -13 Change computation display interval(mm)
226 C          -Input computation display interval(mm)
227 C              range: computation display interval <=100mm
228 C       -14 Show current operating parameters
```

```
C          -Displays current operating parameters
C       -15 Save current operating parameters
C          -Query for name of file which current operatings parameters
C           will be saved. Unit 24 is used.
C       -16 Run program
C           -Executes computational loop until desired termination
C              condition is reached. See below for details.
C       -17 Return to main menu
C           -See above for options in main menu
C       -18 Exit program
C           -Terminates program
C   4-Run program
C      -Executes computational loop until desired termination condition
C           is reached.  See below for details.
C   5-Exit program
C
C -Run program details:
C  -Computation of average molecular weight and gas density
C  -Computation of parameters needed for thermal conductivity and
C     viscosity calculations
C  -computation of channel volumetric flowrate and channel gas velocity
C  -initialize some physical properties parameters
C  -step size computational loop ( 2 loop passes)
C    -compute gas density,channel flow and velocity
C    -compute bulk diffusivity andthermal conductivity
C    -compute viscosity of gas and heat capacity of gas
C    -compute transport parameters and rxn rate
C    -compute thiele modulus and effectiveness factor
C    -compute Reynolds number and conversion
C    -perform Runge-Kutta integration
C    -update variables
C    -return to beginning of step size computational loop
C  -compute step size to produce approx .04% change per loop iteration
C  -initialize some physical properties parameters
C  -main computational loop (continue until termination criteria met)
C    -check if termination criteria are met, if so exit loop
C    -compute gas density,channel flow and velocity
C    -compute bulk diffusivity andthermal conductivity
C    -compute viscosity of gas and heat capacity of gas
C    -compute transport parameters and rxn rate
C    -compute thiele modulus and effectiveness factor
C    -compute Reynolds number and conversion
C    -print(to screen and file) header if first time through
C    -print(to screen and file) parameters at desired interval
C    -perform Runge-Kutta integration
C    -update variables
C    -step size check section, if conversion per step is < 0.08%, then
C      reduce step size (/5) and increase display factor(*5)
C    -parameter value boundary check, if out of bounds, exit loop
C    -return to beginning of main computational loop
C  -final computed values output section
C  -reset some important variable values
C  -return to main menu
C  -end of program
C  -subroutines
C     -RK4, fourth order Runge-Kutta
C     -FUNC, support for RK4
```

```
C     -LINES, writes a specified no. of lines
C     -HEADER, writes a portion of the header to screen and file
C     -TCON, computes thermal cond. of each species and a specifed temp
C     -PROP, computed viscosity and thermal conductivity of gas
C     -VIS, computes the viscosity of each species at a specified temp
C     -OUTPUT, write a portion of the header to screen and file
C     -FXN1, computes effective diffusivity of gas mixture
C     -FXN2, computes heat capacity of gas mixture
C     -FXN3, computes diffusivity of O2 in mixture
C     -FXN4, computes average molecular weight
C

C     PROGRAM LASCAT
C**********Declare variables*********************************************
      COMMON /BLK1/ KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
      COMMON /BLK2/ VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
      INTEGER  FACTOR,ONCE
      REAL*8   MFDH,MCW,MCH,MCWT,CMCWT,MCST,CHWP,CHSTV,CHHD
      REAL*8   TZERO,O2ZERO,MVFLO,CONV,CHFLO,CHGVEL,MONOL,SUM
      REAL*8   CGX,CSX,TGX,TSX,TREF,X,DX,DCGX,DTGX,AREF,A,CDI
      REAL*8   KC,DENGAS,DENGSR,DENCAT,DENSUP,CPGAS,CPCAT,CPSUP
      REAL*8   N,HEATRX,ENGACT,R,THIELE,DAB,DABR,DABEFF,LAMBMX
      REAL*8   H,K,KREF,CONST1,CONST2,CONST3,P,Q,CONVX,ASK
      REAL*8   CONSTD,CONSTE,CONSTF,X0(3),XNEW(3)
      REAL*8   EMICRO,EMACRO,RMICRO,RMACRO,MFDV
      REAL*8   DKMICR,DKMACR,DMICRO,DMACRO
      CHARACTER*1  SS,SSS,SSS1,SSS2,BEEP,CH,CH1,CH2
      CHARACTER*20 FILNAM,S
      REAL*8   T,Y(6),TCONDC,VISCTC,Y10,Y20,Y30,Y40,Y50,Y60
      REAL*8   MW(6),MOLFLO,MVFLZ,PZERO
      REAL*8   VISC(6,2:7),AX(6,6)
      REAL*8   VISCT(6),TCONT(6),AMW,PRESS,D(6),DP
      REAL*8   CONST5,CONST4,CONST6,CONST7,CONST8,CP(6)
      REAL*8   FGX,DFGX,FZERO,FGXEND,NOCHV,NOCHH,NOCHM
      REAL*8   CONVXZ,XZ,CGXZ,CSXZ,TSXZ,RE
      INTEGER I,J,CONSTA,CONSTB,CONSTC, DXCHK,JUMP
      LOGICAL*1 FIRST, MAIN
C******Introduction*************************************************
C     Open Data file which will be used for output.
      OPEN( UNIT=25, FILE='LDATA', STATUS='NEW')
      WRITE(*,*)'            ******     PROGRAM LASCAT     *******'
      WRITE(*,*)
      WRITE(*,*)'    The purpose of this program is to calculate ',
     2 'the gas concentration and'
      WRITE(*,*)'temperature profiles of a monolith catalyst section',
     2 ' of a CO2 laser.  The'
      WRITE(*,*)'CO2 decomposes when the laser is pulsed.  The CO ',
     2 'and O2 produced as a result'
      WRITE(*,*)'of pulsing are detrimental to the efficient opera',
     2'tion of the laser.  The'
      WRITE(*,*)'recombination reaction is CO +1/2 O2 -> CO2.  ',
     2'This program provides the'
      WRITE(*,*)'means to model the performance of a monolith ',
     2'catalyst section under various'
      WRITE(*,*)'gas compositions, temperatures, catalyst ',
     2'activities gas flowrates, oxygen '
      WRITE(*,*)'conversion, monolith face and length dimensions.  ',
```

```
343       2'Results can indicate if '
344        WRITE(*,*)'constraints such as conversion, maximum gas temper',
345       2'ature, monolith weight '
346        WRITE(*,*)'are satisfied and how the system parameters may be',
347       2' altered to meet these'
348        WRITE(*,*)'constraints.  Parameters and options may be altered',
349       2' to tailor the monolith'
350        WRITE(*,*)'design.  Default values can also be used as a ',
351       2'starting point for the design'
352        WRITE(*,*)'process.  A review of the parameters and options',
353       2' chosen may be made prior'
354        WRITE(*,*) 'to execution of the computational portion of the',
355       2' program.'
356        CALL LINES(5)
357        WRITE(*,*)'                          (HIT RETURN TO CONTINUE)'
358        READ(*,621) S
359  621   FORMAT(A)
360  622   FORMAT(A1)
361        BEEP= CHAR(7)
362  C FIRST TIME THROUGH, SKIP OVER QUERY FOR READING PARAMETER FILE
363        GO TO 2119
364  C Default values for parameters
365  C First see if operating parameters are already available in a data
366  C file.
367  9000  WRITE(*,*)
368        WRITE(*,*)'Read in data from existing parameter file ? (Y/N)'
369        READ(*,621) CH
370        IF ((CH.EQ.'Y').OR.(CH.EQ.'y')) THEN
371          WRITE(*,*)
372          WRITE(*,*)
373          WRITE(*,*)'What is the name of the existing parameter file?'
374          WRITE(*,*)'to be opened?'
375          READ(*,621)FILNAM
376          OPEN(UNIT=23, FILE=FILNAM, STATUS='OLD')
377  C If existing data file exists, read in data.
378               READ(23,*)MFDH
379               READ(23,*)MFDV
380               READ(23,*)MCST
381               READ(23,*)MCW
382               READ(23,*)MCH
383               READ(23,*)MCWT
384               READ(23,*)Y(1)
385               READ(23,*)Y(2)
386               READ(23,*)Y(3)
387               READ(23,*)Y(4)
388               READ(23,*)Y(5)
389               READ(23,*)Y(6)
390               READ(23,*)PZERO
391               READ(23,622)SSS
392               READ(23,622)SSS1
393               READ(23,622)SSS2
394               READ(23,*)CONV
395               READ(23,*)MONOL
396               READ(23,*)ENGACT
397               READ(23,*)AREF
398               READ(23,*)TZERO
399               READ(23,*)MVFLZ
```

```
400               READ(23,*)FACTOR
401               READ(23,*)DX
402               READ(23,*)DENCAT
403               READ(23,*)EMICRO
404               READ(23,*)EMACRO
405               READ(23,*)RMICRO
406               READ(23,*)RMACR0
407               CLOSE (UNIT = 23)
408  C If no external data file exists, then assign default values.
409         ELSE
410  2119         WRITE(*,*)
411               WRITE(*,*)' Default values being assigned...'
412  11           MFDH=100.0
413               MFDV=100.0
414               MCST=0.5
415               MCW=4.0
416               MCH=4.0
417               MCWT=0.25
418               Y(1)=0.2
419               Y(2)=0.0000001
420               Y(3)=0.37
421               Y(4)=0.02
422               Y(5)=0.01
423               Y(6)=0.40
424               PZERO=1.0
425               SSS='A'
426               SSS1='P'
427               SSS2='O'
428               CONV=2.5
429               MONOL=5.0
430               ENGACT=39700.0
431               AREF=123.4
432               TZERO=300.0
433               MVFLZ=0.25
434               FACTOR=50
435               DX=0.1
436               DENCAT=5.0E-04
437               EMICRO=0.24
438               EMACRO=0.48
439               RMICRO=1.2E+1
440               RMACRO=5.0E+2
441         ENDIF
442  C Compute a few needed parameters:
443         Y10=Y(1)
444         Y20=Y(2)
445         Y30=Y(3)
446         Y40=Y(4)
447         Y50=Y(5)
448         Y60=Y(6)
449         O2ZERO=100*Y(5)
450         CHWP = 2 * ( MCW + MCH )
451         CHSTV = CHWP / ( MCW * MCH )
452         CHHD = 4 * ( MCW * MCH ) / CHWP
453         NOCHH = (MFDH / (MCH+2*MCST))
454         NOCHV = (MFDV / (MCW+2*MCST))
455         NOCHM = NOCHV * NOCHH
456         CDI=DX*FACTOR
```

```
457 9001  CONTINUE
458 C Set FIRST equal to true the first time through the loop
459 C so that an intial parameters may be viewed.
460       FIRST = .TRUE.
461 C Print Out Main Menu
462       CALL LINES(17)
463       WRITE(*,46)
464 46    FORMAT(1H ,T20,'LASCAT Main Menu')
465       MAIN = .TRUE.
466 9011  WRITE(*,*)
467       WRITE(*,*) '  1) Read in new operating parameters'
468       WRITE(*,*) '  2) Show current operating parameters'
469       WRITE(*,*) '  3) Change operating parameters'
470       WRITE(*,*) '  4) Run program'
471       WRITE(*,*) '  5) Exit program'
472       WRITE(*,*)
473       WRITE(*,*) '     Type in number corresponding to choice above.'
474       CALL LINES(12)
475       ASK=0
476       Read(*,*) ASK
477       IF (ASK.EQ.1) GO TO 9000
478       IF (ASK.EQ.2) GO TO 9002
479       IF (ASK.EQ.3) GO TO 100
480       IF (ASK.EQ.4) GO TO 348
481       IF (ASK.EQ.5) GO TO 99999
482       WRITE(*,*) BEEP, BEEP, BEEP
483       WRITE(*,*)
484       WRITE(*,*)' A number, 1 to 5, is required.'
485       WRITE(*,*)
486       WRITE(*,*)
487       GOTO 9011
488 C Output parameters to screen for review
489 9002  CALL OUTPUT(0,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
490      +            Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
491      +            EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
492      +            CONV,MONOL,DX,CDI)
493       IF (MAIN) THEN
494             GOTO 9001
495       ELSE
496             GOTO 100
497       ENDIF
498 C******Parameter Modification Section**********************************
499 100   MAIN = .FALSE.
500       CALL LINES(9)
501       WRITE(*,73)
502 73    FORMAT(1H ,T20,'Parameter Modification Menu')
503       WRITE(*,*)
504 334   WRITE(*,*)
505       WRITE(*,*) ' 1) Change monolith physical dimensions'
506       WRITE(*,*) ' 2) Change inlet gas composition'
507       WRITE(*,*) ' 3) Change inlet gas volumetric flowrate'
508       WRITE(*,*) ' 4) Change inlet gas temperature'
509       WRITE(*,*) ' 5) Change inlet gas pressure'
510       WRITE(*,*) ' 6) Change catalyst activation energy'
511       WRITE(*,*) ' 7) Change catalyst reaction rate constant'
512       WRITE(*,*) ' 8) Change catalyst active layer density'
513       WRITE(*,*) ' 9) Change macro/micro pore radius & void-fraction'
```

```
514         WRITE(*,*) '10) Change thermal operation (Adiabatic/Isothermal)'
515         WRITE(*,*) '11) Change output profile (Full/ Summary)'
516         WRITE(*,*) '12) Change termination variable (Conversion/Length)'
517         WRITE(*,*) '13) Change computation display interval'
518         WRITE(*,*)
519         WRITE(*,*) '14) Show current operating parameters'
520         WRITE(*,*) '15) Save current operating parameters'
521         WRITE(*,*) '16) Run program'
522         WRITE(*,*) '17) Return to main menu'
523         WRITE(*,*) '18) Exit program'
524         WRITE(*,*)
525         WRITE(*,*) '      Type in number corresponding to choice above'
526         WRITE(*,*)
527         ASK=0
528         READ(*,*) ASK
529         IF (ASK.EQ.1)  GOTO 101
530         IF (ASK.EQ.2)  GOTO 110
531         IF (ASK.EQ.3)  GOTO 120
532         IF (ASK.EQ.4)  GOTO 130
533         IF (ASK.EQ.5)  GOTO 140
534         IF (ASK.EQ.6)  GOTO 150
535         IF (ASK.EQ.7)  GOTO 160
536         IF (ASK.EQ.8)  GOTO 170
537         IF (ASK.EQ.9)  GOTO 180
538         IF (ASK.EQ.10) GOTO 200
539         IF (ASK.EQ.11) GOTO 210
540         IF (ASK.EQ.12) GOTO 220
541         IF (ASK.EQ.13) GOTO 230
542         IF (ASK.EQ.14) GOTO 9002
543         IF (ASK.EQ.15) GOTO 11000
544         IF (ASK.EQ.16) GOTO 348
545         IF (ASK.EQ.17) GOTO 9001
546         IF (ASK.EQ.18) GOTO 99999
547         WRITE(*,*) BEEP, BEEP, BEEP
548         WRITE(*,*)
549         WRITE(*,*)' A number, 1 to 18, is required.'
550         WRITE(*,*)
551         GOTO 334
552 C************* PARAMETER INPUT SECTION************************
553 C INPUT MONOLITH PHYSICAL DIMENSIONS
554 101     WRITE(*,*)
555         MCST=MCST*2.0
556         WRITE(*,*)' Current monolith horizontal '
557         WRITE(*,1075) MFDH
558         WRITE(*,*)
559 1075    FORMAT(' face dimension (mm) =  ',F8.3)
560 1136    WRITE(*,*)' Input new monolith horizontal face dimension.'
561         WRITE(*,*)' Value must be >=10mm and <=1000mm.'
562         READ(*,*) MFDH
563         IF ((MFDH.LT.10.0).OR.(MFDH.GT.1000.0)) GOTO 1136
564         WRITE(*,*)
565         WRITE(*,*)
566         WRITE(*,*)' Current monolith vertical'
567         WRITE(*,1076) MFDV
568 1076    FORMAT(' face dimension (mm) =  ',F8.3)
569         WRITE(*,*)
570         WRITE(*,*)
```

```
1137  WRITE(*,*)' Input new monolith vertical face dimension.'
      WRITE(*,*)' Value must be >=10mm and <=1000mm.'
      READ(*,*) MFDV
      IF ((MFDV.LT.10.0).OR.(MFDV.GT.1000.0)) GOTO 1137
102   WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)' Current monolith channel total'
      WRITE(*,1077) MCST
1077  FORMAT(' wall thicknes (mm) =  ',F8.3)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)' Input the monolith channel total wall'
      WRITE(*,*)' thickness(mm). (Including active layer)'
       READ(*,*)  MCST
       IF (MCST.LE.0.0)   GO TO 102
       IF ((MCST.GE.MFDH).OR.(MCST.GE.MFDV)) THEN
         WRITE(*,*)' Wall thickness must be less than the monolith'
         WRITE(*,*)' face dimension! Right? Let us start over.'
         GOTO 101
       ENDIF
       MCST = MCST / 2.0
103   WRITE(*,*)
      WRITE(*,*)' Current square channel'
      WRITE(*,1078) MCW
1078  FORMAT(' opening dimension (mm) =  ',F8.3)
      WRITE(*,*)
      WRITE(*,*)' Input new monolith square'
      WRITE(*,*)' channel opening dimension(mm).'
       READ(*,*)  MCW
       IF (MCW.LE.0.0)    GO TO 103
       IF ((MCW.GE.MFDH).OR.(MCW.GE.MFDV)) THEN
         WRITE(*,*)' Channel opening must be less than the monolith'
         WRITE(*,*)' face dimension! Right? Let us start over.'
         GOTO 101
       ENDIF
       MCH = MCW
104   WRITE(*,*)
      WRITE(*,*)' Current active layer thickness'
      WRITE(*,1079) MCWT
1079  FORMAT(' thickness (mm) = ',F8.3)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)' Input monolith channel active layer '
      WRITE(*,*)' thickness (mm).  Active layer cannot'
      WRITE(*,1080) MCST*2.00
1080  FORMAT(' be greater than ',F8.3,' (mm),')
      WRITE(*,*)'(1/2 total wall thickness)'
      READ(*,*)  MCWT
      IF ((MCWT.LE.0).OR.(MCWT.GT.MCST))   GO TO 104
      WRITE(*,*)
      WRITE(*,*)
C Perform monolith parameter calculations
8900  CHWP = 2 * ( MCW + MCH )
      CHSTV = CHWP / ( MCW * MCH )
      NOCHH = (MFDH / (MCH+2*MCST))
      NOCHV = (MFDV / (MCW+2*MCST))
      CHHD = 4.0*(MCW*MCH)/CHWP
```

```
628         NOCHM = NOCHV * NOCHH
629         GO TO 100
630   C Input Gas composition
631   C     Define Mole fractions of species Y(i)
632   C     The index of Y(i) correspond to the species.
633   C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
634   110   Write(*,*)' Input section for gas composition:'
635         WRITE(*,*)
636         Write(*,*)' The mixture can consist of only the following'
637         Write(*,*)' species: He, Ar, CO2, CO, O2, N2. All mole '
638         Write(*,*)' fractions must be greater than zero. The sum'
639         WRITE(*,*)' of the mole fractions must be =1'
640         WRITE(*,*)' Current mole fractions: '
641         WRITE(*,3231) Y(1),Y(2),Y(3)
642         WRITE(*,3232) Y(4),Y(5),Y(6)
643   3231  FORMAT('  He = ',F6.4,' Ar = ',F6.4,' CO2 = ',F6.4)
644   3232  FORMAT('  CO = ',F6.4,' O2 = ',F6.4,' N2 = ',F6.4)
645         WRITE(*,*)
646         Write(*,*) 'Input gas mole fraction for He'
647           Read(*,*) Y(1)
648           If (Y(1).EQ.0.0) Y(1)=1E-7
649         Write(*,*) 'Input gas mole fraction for Ar'
650           Read(*,*) Y(2)
651           If (Y(2).EQ.0.0) Y(2)=1E-7
652         Write(*,*) 'Input gas mole fraction for CO2'
653           Read(*,*) Y(3)
654           If (Y(3).EQ.0.0) Y(3)=1E-7
655         WRITE(*,*)
656         Write(*,*) 'Input gas mole fraction for O2'
657         WRITE(*,*)
658         Write(*,*) 'Gas mole fraction for CO will be set to twice that'
659         Write(*,*) 'of O2.  This is because CO and O2 are presumed to'
660         Write(*,*) 'be produced from the dissociation of CO2. '
661         Write(*,*) 'Therefore, the stoichiometric 2:1 ratio applies.'
662         Write(*,*) 'Also, the mole fraction of O2 is limited to a '
663         Write(*,*) 'maximum of 0.03 (3.0%).  Typically a CO2 lasers '
664         Write(*,*) 'output is degraded at a O2 mole fraction of 0.01'
665         Write(*,*) '(1.0%).'
666           Read(*,*) Y(5)
667           IF (Y(5).LE.0.0) THEN
668               Write(*,*) ' There must be O2 to convert !!', BEEP,BEEP
669               Write(*,*) ' Put in a mole fraction > 0'
670               GOTO 110
671           ENDIF
672           IF (Y(5).LT.1E-7) THEN
673               WRITE(*,*) ' Awful low O2 concentration. The problem is'
674               Write(*,*) ' no problem! Put in a mole fraction >= 1E-7'
675               Write(*,*)  BEEP,BEEP
676               GOTO 110
677           ENDIF
678           IF (Y(5).GT.0.0300001) THEN
679               Write(*,*) ' Awful high O2 concentration, The laser'
680               Write(*,*) ' may explode! Shut it off immediately'
681               Write(*,*)  BEEP,BEEP
682               Write(*,*) ' Put in a mole fraction <= 0.03 '
683               GOTO 110
684           ENDIF
```

```
685           Y(4)=2.0*Y(5)
686           O2ZERO=Y(5)*100
687         Y(6) = 1.0-Y(5)-Y(4)-Y(3)-Y(2)-Y(1)
688         IF ((Y(6).LT.0.0).OR.(Y(6).GT.1.0)) GOTO 110
689         IF ((Y(6).LT.1E-7).AND.(Y(6).GE.0)) Y(6)=1E-7
690         WRITE(*,*)
691  C Check if restrictions are met.If not, force user to reinput values
692               Do 112 I=1,5
693                 IF ((Y(I).LT.0).or.(Y(I).GT.1.0)) THEN
694                   WRITE(*,*) BEEP,BEEP
695                   WRITE(*,*)' Invalid mole fractions. Try again.'
696                   WRITE(*,*)' Restrictions are not met. Read below'
697                   Write(*,*)
698                   GOTO 110
699                 ENDIF
700  112          Continue
701         WRITE(*,2323) Y(6)
702  2323   FORMAT(' The gas mole fraction for N2 = ',F6.4)
703         Y10=Y(1)
704         Y20=Y(2)
705         Y30=Y(3)
706         Y40=Y(4)
707         Y50=Y(5)
708         Y60=Y(6)
709         WRITE(*,*)
710         WRITE(*,*)
711         WRITE(*,*)'     ==> Hit Return when Finished Viewing <=='
712         WRITE(*,*)
713         READ(*,621) S
714         WRITE(*,*)
715         WRITE(*,*)
716         GO TO 100
717  C Input Inlet gas flowrate
718  120    WRITE(*,*)
719         WRITE(*,*)' Current inlet volumetric'
720         WRITE(*,1081) MVFLZ
721  1081   FORMAT(' flowrate = ',F8.3,' (l/s).')
722         WRITE(*,*)
723         WRITE(*,*)' Input monolith inlet volumetric flowrate.'
724          READ(*,*)  MVFLZ
725          IF (MVFLZ.LE.0.0)  GO TO 120
726         GO TO 100
727  C Input Inlet gas temperature
728  130    WRITE(*,*)
729         WRITE(*,*)' Current inlet gas '
730         WRITE(*,1082) TZERO
731  1082   FORMAT(' temperature = ',F8.3,' (K),')
732         WRITE(*,*)
733         WRITE(*,*)'Input monolith inlet gas temperature.'
734         WRITE(*,*)'Temperature must be >200K and <700K.'
735          READ(*,*)  TZERO
736          IF ((TZERO.EQ.0).OR.(TZERO.LT.200)) GO TO 130
737          IF (TZERO.GT.700)  GO TO 130
738          GOTO 100
739  C Input Inlet Gas Pressure
740  140    WRITE(*,*)
741         PZERO=PZERO*101.325
```

```
742         WRITE(*,*)' Current inlet gas '
743         WRITE(*,1083) PZERO
744  1083   FORMAT(' pressure = ',F8.3,' (kPa)')
745         WRITE(*,*)
746         WRITE(*,*)' Inlet gas pressure must be between'
747         WRITE(*,*)' 0.1 and 350 kPa'
748         WRITE(*,*)' Input new inlet gas pressure.'
749         READ(*,*) PZERO
750         IF ((PZERO.LT.0.1).OR.(PZERO.GT.350.0)) GOTO 140
751  C      convert pressure back to atm.
752         PZERO=PZERO/101.325
753         GOTO 100
754  C Input catalyst activation energy
755  150    WRITE(*,*)
756         WRITE(*,1084) ENGACT
757  1084   FORMAT(' Current activation energy = ',F11.3,' (J/mol),')
758         WRITE(*,*)' Maximum activation energy (J/mol) = 300000'
759         WRITE(*,*)
760         WRITE(*,*)' Catalyst activation energy(J/mol)'
761          READ(*,*)  ENGACT
762          IF ((ENGACT.LE.0.0).OR.(ENGACT.GT.300000))  GOTO 150
763         GO TO 100
764  C Input catalyst reaction rate constant
765  160    WRITE(*,*)
766         WRITE(*,*)' Current catalyst reaction rate'
767         WRITE(*,1085) AREF
768  1085   FORMAT(' constant [@ 298 K] = ',F11.3,' (mm^3/gcat-s),')
769         WRITE(*,*)
770         WRITE(*,*)' Input new catalyst reaction'
771         WRITE(*,*)' rate constant at 298 K (mm^3/gcat-s)'
772         WRITE(*,*)' Rate must be greater than zero'
773          READ(*,*)  AREF
774          IF (AREF.LE.0.0)  GOTO 160
775         GO TO 100
776  C Input catalyst active layer density
777  170    WRITE(*,*)
778         WRITE(*,*)'Current density of catalyst'
779         WRITE(*,1086) DENCAT
780  1086   FORMAT(' active layer = ',E10.4,' (g/mm^3),')
781         WRITE(*,*)
782         WRITE(*,*)'Input density of catalyst active layer (g/mm^3)'
783         WRITE(*,*)'Density must be greater than zero'
784         READ(*,*) DENCAT
785         IF (DENCAT.LE.0.0) GOTO 170
786         WRITE(*,*)
787         GOTO 100
788  C Input micro/macropore radii and void-fractions
789  180    WRITE(*,*)
790         WRITE(*,*)' Current average micropore  '
791         WRITE(*,1087) RMICRO
792  1087   FORMAT(' radius = ',F9.4,' (nm),')
793         WRITE(*,*)' Input new average micropore radius (nm)'
794         WRITE(*,*)' Micro radius must be greater than zero'
795         READ(*,*) RMICRO
796         WRITE(*,*)
797         WRITE(*,*)' Current average macropore'
798         WRITE(*,1088) RMACRO
```

```
1088  FORMAT(' radius = ',F9.4,' (nm),')
      WRITE(*,*)' Input new average macropore radius (nm)'
      WRITE(*,*)' Macro radius must be greater than zero'
      READ(*,*) RMACRO
      WRITE(*,*)
      IF ((RMICRO.LE.0.0).OR.(RMACRO.LE.0.0)) GO TO 180
      IF(RMICRO.GT.RMACRO) THEN
            WRITE(*,*)' Hey Dude, What`s the deal?'
            WRITE(*,*)' You just entered macropore radius which is'
            WRITE(*,*)' smaller than the micropore radius!! '
            WRITE(*,*)' Try again, big guy !!'
            WRITE(*,*)
            GOTO 180
      ENDIF
190   WRITE(*,1089) EMICRO
      WRITE(*,1090) EMACRO
1089  FORMAT(' Current void-fraction as micropores ', F6.3)
1090  FORMAT(' Current void-fraction as macropores ', F6.3)
      WRITE(*,*)
      WRITE(*,*)' The sum of micro and macropore void-fractions'
      WRITE(*,*)' must be less than one (1) '
      WRITE(*,*)' Void fractions must be >=0 and <=1'
      WRITE(*,*)
      WRITE(*,*)' Input void-fraction as micropores '
      READ(*,*) EMICRO
      WRITE(*,*)' Input void-fraction as macropores '
      READ(*,*) EMACRO
      WRITE(*,*)
      IF((EMICRO.LT.0.0).OR.(EMACRO.LT.0.0)) THEN
            WRITE(*,*)' You can`t have a negative void fraction'
            WRITE(*,*)
            WRITE(*,*)
            GOTO 190
      ENDIF
      IF (EMICRO+EMACRO.GT.1.0) THEN
            WRITE(*,*)' The sum of micro and macropore void'
            WRITE(*,*)' fractions must be less than one (1) '
            WRITE(*,*)
            GOTO 190
      ENDIF
      WRITE(*,*)
      GOTO 100
C Input thermal opearation: adiabatic or isothermal
200   IF (SSS.EQ.'I') THEN
            WRITE(*,*)' Current operation is isothermal'
      ELSE
            WRITE(*,*)' Current operation is adiabatic'
      END IF
      WRITE(*,*)
      WRITE(*,*)'Isothermal (I) or Adiabatic (A) operation?'
      WRITE(*,*)'Type the letter I or the letter A. HIT RETURN'
      READ(*,621)  SSS
      IF (SSS.EQ.'i') SSS = 'I'
      IF (SSS.EQ.'a') SSS = 'A'
      IF ((SSS.NE.'I').AND.( SSS.NE.'A')) GOTO 200
      GO TO 100
C Input output profile type: full or summary
```

```
856 210   WRITE(*,*)
857       WRITE(*,*)' Full concentration and temperature profile (P) or'
858      2'summary(S)?'
859       WRITE(*,*)'Type the letter P or the letter S. HIT RETURN. '
860       READ(*,621)  SSS1
861       IF (SSS1.EQ.'p') SSS1 = 'P'
862       IF (SSS1.EQ.'s') SSS1 = 'S'
863       IF ((SSS1.NE.'P').AND.( SSS1.NE.'S')) GO TO 210
864       GO TO 100
865 C Input computation loop completion criteria
866 220   WRITE(*,*)
867       WRITE(*,*)' Integration can be stopped by either specifying'
868       WRITE(*,*)' an amount of O2 conversion (O), or by specifying'
869       WRITE(*,*)' a monolith length (L)'
870       WRITE(*,*)
871       IF (SSS2 .EQ. 'O') THEN
872          WRITE(*,*)' Currently, Integration will be stopped'
873          WRITE(*,*)' by specifying an amount of O2 conversion (O).'
874       ELSE
875          WRITE(*,*)' Currently, Integration will be stopped'
876          WRITE(*,*)' by specifying a monolith length (L).'
877       END IF
878       WRITE(*,*)
879       WRITE(*,*)' Type the letter O or the letter L. HIT RETURN.'
880       READ(*,621)  SSS2
881       IF(SSS2.EQ.'o') SSS2 = 'O'
882       IF(SSS2.EQ.'l') SSS2 = 'L'
883       IF ((SSS2.NE.'O').AND.( SSS2.NE.'L')) GO TO 220
884       IF (SSS2.EQ.'O') THEN
885 225         IF (MONOL.EQ.0) THEN
886                WRITE(*,*)
887                WRITE(*,1091) CONV
888 1091  FORMAT(' Current % oxygen conversion = ',F8.3)
889         END IF
890         WRITE(*,*)
891         WRITE(*,*)' Input desired % oxygen conversion'
892         WRITE(*,*)' between 0 and 100%.'
893         READ(*,*) CONV
894         IF ((CONV.GT.100.0).OR.(CONV.LT.0)) GOTO 225
895       ENDIF
896 227   IF (SSS2.EQ.'L') THEN
897         WRITE(*,*)
898         WRITE(*,1092) MONOL
899 1092  FORMAT(' Current desired monolith length = ',F8.3,' (mm)')
900         WRITE(*,*)
901         WRITE(*,*)' Input desired monolith length (5-4000mm)'
902         WRITE(*,*)
903          READ(*,*) MONOL
904         IF (MONOL.LT.5.0) GOTO 227
905         IF (MONOL.GT.4000.0) GOTO 227
906       ENDIF
907       GO TO 100
908 C Input computation loop(integration) step size ***
909 230   WRITE(*,*)
910       WRITE(*,1093) CDI
911 1093  FORMAT(' Current computation display interval ', F6.3,' (mm)')
912       WRITE(*,*)' Minimum computation display interval = 0.001 mm.'
```

```
913         WRITE(*,*)' Maximum computation display interval = 100 mm.'
914         WRITE(*,*)' Values > 1 will be rounded to the nearest integer'
915         WRITE(*,*)
916         WRITE(*,*)' Input desired computation display interval (mm).'
917         WRITE(*,*)
918         WRITE(*,*)
919          READ(*,*) CDI
920          IF (CDI.GT.100) GOTO 230
921          IF (CDI.GT.1.0) CDI=INT(CDI)
922          IF (CDI.LT.0.0009999) GOTO 230
923         WRITE(*,*)
924         WRITE(*,*)
925         GO TO 100
926  C END of parameter input section
927  C Save present operationg parameters to file
928  11000  WRITE(*,*)
929  C      Give user option to save current operating parameters.
930         WRITE(*,*)
931         WRITE(*,*)' Would you like to save the current operating'
932         WRITE(*,*)' parameters to a New(N) or Existing(E) file?'
933         WRITE(*,*)
934           READ(*,621) CH1
935           IF((CH1.NE.'E').AND.(CH1.NE.'e').AND.(CH1.NE.'N')
936       *      .AND.(CH1.NE.'n')) GOTO 11000
937            IF ((CH1.EQ.'E').OR.(CH1.EQ.'e')) THEN
938                  WRITE(*,*)
939                  WRITE(*,*)'What`s the name of the EXISTING'
940                  WRITE(*,*)'parameter file to be opened?'
941                  READ(*,621) FILNAM
942                  OPEN( UNIT=24, FILE=FILNAM, STATUS='OLD')
943            ELSE
944                  WRITE(*,*)
945                  WRITE(*,*)'What`s the name of the NEW'
946                  WRITE(*,*)'parameter file to be opened?'
947                  READ(*,621) FILNAM
948                  OPEN( UNIT=24, FILE=FILNAM, STATUS='NEW')
949            ENDIF
950  C Write default parameters to parameter file.
951            WRITE(24,*)MFDH
952            WRITE(24,*)MFDV
953            WRITE(24,*)MCST
954            WRITE(24,*)MCW
955            WRITE(24,*)MCH
956            WRITE(24,*)MCWT
957            WRITE(24,*)Y(1)
958            WRITE(24,*)Y(2)
959            WRITE(24,*)Y(3)
960            WRITE(24,*)Y(4)
961            WRITE(24,*)Y(5)
962            WRITE(24,*)Y(6)
963            WRITE(24,*)PZERO
964            WRITE(24,622)SSS
965            WRITE(24,622)SSS1
966            WRITE(24,622)SSS2
967            WRITE(24,*)CONV
968            WRITE(24,*)MONOL
969            WRITE(24,*)ENGACT
```

```
970               WRITE(24,*)AREF
971               WRITE(24,*)TZERO
972               WRITE(24,*)MVFLZ
973               WRITE(24,*)FACTOR
974               WRITE(24,*)DX
975               WRITE(24,*)DENCAT
976               WRITE(24,*)EMICRO
977               WRITE(24,*)EMACRO
978               WRITE(24,*)RMICRO
979               WRITE(24,*)RMACRO
980               CLOSE ( UNIT = 24)
981         GOTO 100
982   C COMPUTE  GAS AVG. MOLECULAR WEIGHT AND DENSITY *
983   348   AMW = FXN4(Y)
984         R=8.3144
985         DENGAS=AMW*(PZERO/9896.0)/R/TZERO
986   C Parameters needed for thermal cond. calcuation
987   C     Read in viscosity (VISC) values into matrix. Units for
988   C     VISC are centipoises. The values are read off a nomagraph
989   C     in Perry's Chemical Engineering Handbook, 5th ed., p3-210.
990   C     The first index of VISC corresponds to the species.
991   C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
992   C     The second index of VISC corresponds to the temperature.
993   C     Temperature:  2=200K,3=300K,4=400K,5=500K,6=600K,7=700K
994         DATA VISC(1,2),VISC(1,3),VISC(1,4),VISC(1,5),VISC(1,6),VISC(1,7)
995        +/.014,.0188,.022,.027,.031,.034/
996         DATA VISC(2,2),VISC(2,3),VISC(2,4),VISC(2,5),VISC(2,6),VISC(2,7)
997        +/.0164,.0223,.0278,.0327,.0376,.041/
998         DATA VISC(3,2),VISC(3,3),VISC(3,4),VISC(3,5),VISC(3,6),VISC(3,7)
999        +/.0105,.0147,.019,.023,.027,.031/
1000        DATA VISC(4,2),VISC(4,3),VISC(4,4),VISC(4,5),VISC(4,6),VISC(4,7)
1001       +/.0138,.018,.022,.0255,.029,.0325/
1002        DATA VISC(5,2),VISC(5,3),VISC(5,4),VISC(5,5),VISC(5,6),VISC(5,7)
1003       +/.0155,.02,.0247,.0288,.0327,.0368/
1004        DATA VISC(6,2),VISC(6,3),VISC(6,4),VISC(6,5),VISC(6,6),VISC(6,7)
1005       +/.013,.0175,.0218,.026,.029,.0332/
1006        MVFLO=MVFLZ
1007  C CONVERT MVFLO FROM liters/s TO mm^3/s
1008        MVFLO = MVFLO *1.0E+06
1009  C COMPUTE MOLAR FLOWRATE OF GAS. (M/s)
1010        MOLFLO = MVFLO*DENGAS*AMW
1011  C COMPUTE CHANNEL FLOW RATE AND CHANNEL VELOCITY
1012        CHFLO = MVFLO / NOCHM
1013        CHGVEL = CHFLO / ( MCW * MCH)
1014  349   CONTINUE
1015
1016  C INTIALIZE PHYSICAL PROPERTIES PARAMETERS
1017  1041  HEATRX=5.64E+05
1018        TREF=298.0
1019        PRESS = PZERO
1020        TGX= TZERO
1021        TSX= TZERO
1022        CGX= 4.092E-08 * (O2ZERO/100.0)*(298.0/TGX)*(PRESS/1.0)
1023        FGX=CGX*CHFLO
1024        FZERO=FGX
1025        FGXEND=FZERO*(1.0 - CONV/100.0)
1026        S = CHAR(9)
```

```
1027        SS = CHAR(13)
1028        X=0.0
1029        CMCWT= ((MCH+2*MCWT)*(MCW+2*MCWT)-(MCH*MCW))/2/(MCH+MCW)
1030        CONSTA=0.0
1031        DCGX=0.0
1032        DFGX=0.0
1033        ICNT = 0
1034  C Initialize variables for Runge Kutta Integration method
1035        XNEW(1) = FGX
1036        XNEW(2) = PZERO
1037        XNEW(3) = TZERO
1038
1039  C************* START OF STEP SIZE CHECK LOOP *********************
1040  1060  DO 8001 P=0,2
1041        DX=1E-6
1042        DENGAS=AMW*(PRESS/9896.0)/R/TGX
1043  C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY
1044        MVFLO = MOLFLO / (AMW * DENGAS)
1045        CHFLO = MVFLO / NOCHM
1046        CHGVEL = CHFLO / ( MCW * MCH)
1047  C COMPUTE BULK DIFFUSIVITY
1048        DAB = FXN3(Y,TGX)
1049  C COMPUTE EFFECTIVE DIFFUSIVITY
1050        DABEFF= FXN1(DAB,Y(5),PRESS,RMICRO,RMACRO,
1051       + TSX,EMACRO,EMICRO)
1052  C COMPUTE THERMAL CONDUCTIVITY
1053        T=TGX
1054  C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX
1055        CALL VIS(TGX,VISC,VISCT)
1056  C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1057        CALL TCON(TGX,TCONT)
1058  C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1059        CALL PROP(Y,TCONT,VISCT,VISCTC,K)
1060  C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1061        CPGAS=FXN2(Y,TGX)
1062        KC = 2.976 * DAB / CHHD
1063        H = 2.976 * K / CHHD
1064        A = AREF * DEXP ( -ENGACT / R * ( 1 / TSX -1 / TREF))
1065        THIELE = CMCWT * (  A  * DENCAT / DABEFF) ** 0.5
1066        N = DTANH ( THIELE ) / THIELE
1067        CONST1= N*A*CMCWT*DENCAT
1068        CSX = CGX * ( KC) / (KC+CONST1)
1069        TSX =TGX + HEATRX*CSX*CONST1/H
1070  C FIRST TIME THROUGH COMPUTE 'A' TO USE FOR TSX,CSX CALCULATION
1071        IF (FIRST.EQ..TRUE.) THEN
1072              A = AREF * DEXP ( -ENGACT / R * ( 1 / TSX -1 / TREF))
1073              THIELE = CMCWT * (  A  * DENCAT / DABEFF) ** 0.5
1074              N = DTANH ( THIELE ) / THIELE
1075              CONST1= N*A*CMCWT*DENCAT
1076              CSX = CGX * ( KC) / (KC+CONST1)
1077              TSX =TGX + HEATRX*CSX*CONST1/H
1078              IF (SSS.EQ.'I') TSX=TGX
1079              IF (P.EQ.0) THEN
1080                    XZ=0
1081                  CONVXZ=0.0
1082                  CGXZ=CGX
1083                  CSXZ=CSX
```

```
1084                    TSXZ=TSX
1085                ENDIF
1086          ENDIF
1087          RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1088          CONVX = 100.0*(CGXZ-CGX*TGX/TZERO*PZERO/PRESS)/CGXZ
1089 C Reset variables each time Runge Kutta Subroutine is called
1090 7889    X0(1) = XNEW(1)
1091          X0(2) = XNEW(2)
1092          X0(3) = XNEW(3)
1093 C Call Runge Kutta Subroutine:
1094          CALL RK4(DX,X,X0,XNEW)
1095 C PARMETER UPDATE
1096          FGX = XNEW(1)
1097          PRESS = XNEW(2)
1098          IF (SSS.EQ.'I')  THEN
1099                TGX = TZERO
1100          ELSE
1101                TGX = XNEW(3)
1102          ENDIF
1103          CGX = FGX/CHFLO
1104          X   = X +  DX
1105          Y(5)=Y50*(100.0-CONVX)/100.0
1106          Y(4)=Y40-2*(Y50-Y(5))
1107          Y(3)=Y30+2*(Y50-Y(5))
1108          Y(1)=Y10
1109          Y(2)=Y20
1110          Y(6)=Y60
1111          CONST7 = Y(1) + Y(2) + Y(3) + Y(4)+ Y(5)+ Y(6)
1112          DO 33446 JJ=1,6
1113             Y(JJ)=Y(JJ)/CONST7
1114 33446 CONTINUE
1115 8001  CONTINUE
1116 C************** END OF STEP SIZE CHECK LOOP ********************
1117
1118
1119
1120 C CALCULATE STEP SIZE AND DISPLAY FACTOR USING COMPUTATIONAL
1121 C DISPLAY FACTOR AND CONVX CALCULATED IN STEP SIZE CHECK LOOP
1122          DX=1E-6*0.04/CONVX
1123          IF (DX.GT.5) DX=5
1124          IF (DX.LT.0.1E-4)  DX=0.1E-4
1125          IF (CDI.LT.DX) DX=CDI
1126 2345  FACTOR=INT(CDI/DX)
1127          IF (FACTOR.GE.250) THEN
1128                CDI=CDI*250/FACTOR
1129                FACTOR=250
1130          ENDIF
1131          DX=CDI/FACTOR
1132 C INITIALIZE PARAMETERS FOR MAIN COMPUTATIONAL LOOP
1133          PRESS = PZERO
1134          TGX= TZERO
1135          TSX= TZERO
1136          CGX= 4.092E-08 * (O2ZERO/100.0)*(298.0/TGX)*(PRESS/1.0)
1137          FGX=CGX*CHFLO
1138          FZERO=FGX
1139          FGXEND=FZERO*(1.0 - CONV/100.0)
1140          CGXTMP=CGX
```

```
1141        X=0.0
1142        CONSTA=0.0
1143        DCGX=0.0
1144        DFGX=0.0
1145        ICNT = 0
1146        TGNEW=TZERO
1147        MVFLO=MVFLZ
1148          Y(1)=Y10
1149          Y(2)=Y20
1150          Y(3)=Y30
1151          Y(4)=Y40
1152          Y(5)=Y50
1153          Y(6)=Y60
1154  C Initialize variables for Runge Kutta Integration method
1155        XNEW(1) = FGX
1156        XNEW(2) = PZERO
1157        XNEW(3) = TZERO
1158        JUMP=0
1159        ONCE=0
1160
1161
1162  C************* START OF MAIN COMPUTATIONAL LOOP *********************
1163  1059  DO 8000 P=0,100000
1164        IF ((DCGX.GT.0.0).OR.(CGX.LT.0.0)) THEN
1165          WRITE(*,*)' Something is wrong, conversion is proceeding'
1166          WRITE(*,*)' in the wrong direction or the concentration'
1167          WRITE(*,*)' of O2 has dropped below zero.'
1168          WRITE(*,*)' Try a lower computation display increment.'
1169          WRITE(*,*)' Try a lower gas inlet temperature or flowrate.'
1170          WRITE(*,*)
1171          WRITE(*,*)' Change in conc of O2 per step(DCGX) = ',DCGX
1172          WRITE(*,*)' O2 concentration(CGX) = ',CGX
1173          WRITE(*,*)
1174          GOTO 17000
1175        ENDIF
1176  C Check to see if conversion has been reached.
1177        IF (SSS2.EQ.'O') THEN
1178            IF ((CONVX.GE.CONV)) GOTO 9900
1179        ELSE
1180            IF (X.GT. MONOL) GOTO 9900
1181        ENDIF
1182  C COMPUTE  GAS AVG. MOLECULAR WEIGHT AND DENSITY
1183  8250  AMW = FXN4(Y)
1184        DENGAS=AMW*(PRESS/9896.0)/R/TGX
1185  C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY
1186        MVFLO = MOLFLO / (AMW * DENGAS)
1187        CHFLO = MVFLO / NOCHM
1188        CHGVEL = CHFLO / ( MCW * MCH)
1189  C COMPUTE BULK DIFFUSIVITY OF O2
1190        DAB = FXN3(Y,TGX)
1191  C COMPUTE EFFECTIVE DIFFUSIVITY OF MIXTURE AT TSX
1192        DABEFF= FXN1(DAB,Y(5),PRESS,RMICRO,RMACRO,
1193       + TSX,EMACRO,EMICRO)
1194        IF (MOD( CONSTA,4) .GT. 0.0 ) GO TO 6669
1195          T=TGX
1196  C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX
1197        CALL VIS(TGX,VISC,VISCT)
```

```
1198 C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1199       CALL TCON(TGX,TCONT)
1200 C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1201       CALL PROP(Y,TCONT,VISCT,VISCTC,K)
1202 6666  CONTINUE
1203 C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1204       CPGAS=FXN2(Y,TGX)
1205 C Limiting Nu and Sh numbers are 2.976.  This is taken from page
1206 C 241 of Convective Heat Transfer by Burmeister, L. C., John
1207 C Wiley & Sons, (1983).  This assumes a constant temperature
1208 C profile(Nu) or concentration profile(Sh).
1209 6669  KC = 2.976 * DAB / CHHD
1210       H = 2.976 * K / CHHD
1211       A = AREF * DEXP(-ENGACT/ R *(TREF-TSX)/TSX/TREF)
1212       THIELE = CMCWT * DSQRT(  A  * DENCAT / DABEFF)
1213       IF ((THIELE.GT.100.0).AND.(ONCE.NE.1)) THEN
1214        WRITE(*,*) 'THEILE MODULUS IS > 100.  SETTING THIELE=100'
1215        WRITE(*,*) 'TO PREVENT NUMERIC OVERFLOW ERROR'
1216        ONCE=1
1217       ENDIF
1218       IF ((THIELE.GT.100.0)) THIELE=100.0
1219       N = DTANH ( THIELE ) / THIELE
1220       CONST1= N*A*CMCWT*DENCAT
1221       CSX = CGX * ( KC) / (KC+CONST1)
1222       TSX =TGX + HEATRX*CSX*CONST1/H
1223       IF (FIRST.EQ..TRUE.) THEN
1224         A = AREF*DEXP(-ENGACT/ R*(TREF-TSX)/TSX/TREF)
1225         THIELE = CMCWT * DSQRT(  A  * DENCAT / DABEFF)
1226         N = DTANH ( THIELE ) / THIELE
1227         CONST1= N*A*CMCWT*DENCAT
1228         CSX = CGX * ( KC) / (KC+CONST1)
1229         TSX =TGX + HEATRX*CSX*CONST1/H
1230         IF (SSS.EQ.'I') TSX=TGX
1231         IF (P.EQ.0) THEN
1232         XZ=0
1233         CONVXZ=0.0
1234         CGXZ=CGX
1235         CSXZ=CSX
1236         TSXZ=TSX
1237       ENDIF
1238       ENDIF
1239       RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1240       CONVX = 100.0*(CGXZ-CGX*TGX/TZERO*PZERO/PRESS)/CGXZ
1241 C HEADER OUTPUT SECTION
1242 C Print out Reynold's number the first time through the loop.
1243 C If First = .true. then print out reynold's number, else don't
1244 C worry about it. Also, print out header and results at position X=0
1245       IF (FIRST.EQ..TRUE.) THEN
1246 C Output of selectable parameter to data file
1247       CALL OUTPUT(1,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
1248      +            Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
1249      +            EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
1250      +            CONV,MONOL,DX,CDI)
1251       CALL HEADER(0,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1252      + DABEFF,PRESS,Y,DX)
1253       FIRST=.FALSE.
1254       WRITE(*,*)
```

```
1255        WRITE(25,*)
1256        WRITE(*,9950)
1257        WRITE(25,9950)
1258        WRITE(*,9951)
1259        WRITE(25,9951)
1260  9950  FORMAT(' Distance',1X,'%Conver',2X,'O2gas',4X,'O2wall',2X,
1261       +'O2center',3X,'Tgas',5X,'Twall',3X,'DPress')
1262  9951  FORMAT('    (mm)',11X,'(mMOL/L)',1X,'(mMOL/L)',1X,'(mMOL/L)',
1263       +1X,'(Kelvin)',1X,'(Kelvin)',3X,'(kPa)')
1264        WRITE(*,*)
1265        WRITE(25,*)
1266        WRITE(*,10) XZ,CONVXZ,CGXZ*1E+09,CSXZ*1E+09,
1267       +(CSXZ*1E+09/DCOSH(THIELE)),TZERO,TSXZ,(PZERO-PZERO)*101.325
1268        WRITE(25,20) XZ,S,CONVXZ,S,CGXZ*1E+09,S,CSXZ*1E+09,S,
1269       +(CSXZ*1E+09/DCOSH(THIELE)),S,TZERO,S,TSXZ,S,
1270       +(PZERO-PZERO)*101.325
1271  10    FORMAT(F8.3,1X,F8.4,1X,F7.4,1X,F7.4,1X,F7.4,5X,F7.3,1X,F8.3
1272       +,1X,E10.3)
1273  20    FORMAT(F8.3,A1,F8.4,A1,F7.4,A1,F7.4,A1,F7.4,A1,F7.3,A1,F8.3
1274       +,A1,E10.3)
1275        ELSE
1276
1277  C COMPUTED VALUES OUTPUTTED TO SCREEN AND FILE AT DISPLAY INTERVAL
1278  C WRITE RESULTS TO SCREEN WHEN REMAINDER OF CONSTA/FACTOR > 0
1279  C ELSE, JUST CALCULATE VALUES AND DON'T PRINT THEM OUT.
1280         IF (MOD(CONSTA,FACTOR).GT.0.0) GOTO 7777
1281         IF (SSS1 .EQ.'S') GOTO 7777
1282         IF (SSS.EQ.'I') TSX=TGX
1283        WRITE(*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
1284       +(CSX*1E+09/DCOSH(THIELE)),TGX,TSX,(PRESS-PZERO)*101.325
1285        WRITE(25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1286       +(CSX*1E+09/DCOSH(THIELE)),S,TGX,S,TSX,S,
1287       +(PRESS-PZERO)*101.325
1288  7777  ENDIF
1289  C Reset variables each time Runge Kutta Subroutine is called
1290  7888   X0(1) = XNEW(1)
1291         X0(2) = XNEW(2)
1292         X0(3) = XNEW(3)
1293  C Call Runge Kutta Subroutine:
1294        CALL RK4(DX,X,X0,XNEW)
1295  C PARMETER UPDATE SECTION
1296        FGX = XNEW(1)
1297        PRESS = XNEW(2)
1298        IF (SSS.EQ.'I')  THEN
1299              TGX = TZERO
1300        ELSE
1301              TGX = XNEW(3)
1302        ENDIF
1303        CGX = FGX/CHFLO
1304        DCGX=CGX-CGXTMP
1305        X    = X +  DX
1306        CGXTMP=CGX
1307        Y(5)=Y50*(100.0-CONVX)/100.0
1308        Y(4)=Y40-2*(Y50-Y(5))
1309        Y(3)=Y30+2*(Y50-Y(5))
1310        Y(1)=Y10
1311        Y(2)=Y20
```

```
1312        Y(6)=Y60
1313        CONST7 = Y(1) + Y(2) + Y(3) + Y(4)+ Y(5)+ Y(6)
1314        DO 33445 JJ=1,6
1315          Y(JJ)=Y(JJ)/CONST7
1316  33445 CONTINUE
1317  C ADAPTIVE STEP SIZE SECTION
1318        IF(((-100.*DCGX/CGX.GT..08)).AND.(JUMP.LT.1)) THEN
1319          DX = DX/5.0
1320          FACTOR = FACTOR*5
1321          IF (DX.LT. 1E-4) JUMP=1
1322          CONSTA=FACTOR-1
1323          WRITE(*,*)  'Reduced step size to ', DX,' mm'
1324        ENDIF
1325        CONSTA=CONSTA + 1
1326  C PARAMETER BOUNDARY CHECK
1327  C     Check to make sure that Temperature, Pressure, and Reynold's
1328  C     number are still in valid range.
1329  C     Temperature must be between 200-700 K
1330  C     Pressure must be between 10E-03 and 3.45 bar
1331  C     Reynolds number must be in laminar region. < 2300
1332              IF (TGX.GT.700.0)  THEN
1333                    WRITE(*,*)
1334                    WRITE(*,*)' Current Gas Temperature = ',TGX
1335                    WRITE(*,*)
1336                    WRITE(*,*)' Error:'
1337                    WRITE(*,*)' This value exceeds the allowable'
1338                    WRITE(*,*)' maximum temperature of 700 K'
1339                    WRITE(*,*)' Lower the inlet gas temperature.'
1340                    WRITE(*,*)
1341                    WRITE(*,*) 'Hit Return When Finished Viewing'
1342                    WRITE(*,*)
1343                    READ(*,621) S
1344                    WRITE(*,*)
1345                    WRITE(*,*)
1346                    GOTO 7564
1347              ELSE IF(RE.GT.2300.0) THEN
1348                    WRITE(*,*)
1349                    WRITE(*,*)' Current Reynolds number = ',RE
1350                    WRITE(*,*)
1351                    WRITE(*,*)' Error:'
1352                    WRITE(*,*)' This value exceeds the maximum'
1353                    WRITE(*,*)' allowable Reynolds number of 2300.'
1354                    WRITE(*,*)' Reduce the inlet gas flowrate.'
1355                    WRITE(*,*)
1356                    WRITE(*,*) 'Hit Return When Finished Viewing'
1357                    WRITE(*,*)
1358                    READ(*,621) S
1359                    WRITE(*,*)
1360                    WRITE(*,*)
1361                    GOTO 7564
1362              ELSE IF((TGX.LT.200.0)) THEN
1363                    WRITE(*,*)
1364                    WRITE(*,*)' Current Gas Temperature = ',TGX
1365                    WRITE(*,*)
1366                    WRITE(*,*)' Error:'
1367                    WRITE(*,*)' This value is less than the minimum'
1368                    WRITE(*,*)' allowable Temperature of 200 K.'
```

```
1369                    WRITE(*,*)' Raise the inlet gas temperature.'
1370                    WRITE(*,*)
1371                    WRITE(*,*) 'Hit Return When Finished Viewing'
1372                    WRITE(*,*)
1373                    READ(*,621) S
1374                    WRITE(*,*)
1375                    WRITE(*,*)
1376                    GOTO 7564
1377               ELSE IF(PRESS*101.325.GT.350.0) THEN
1378                    WRITE(*,*)
1379                   WRITE(*,*)'Current Pressure= ',PRESS*101.325,' kPa'
1380                    WRITE(*,*)
1381                    WRITE(*,*)' Error:'
1382                    WRITE(*,*)' This value exceeds the maximum '
1383                    WRITE(*,*)' allowable Pressure of 350 kPa.'
1384                    WRITE(*,*)' Reduce the inlet gas pressure.'
1385                    WRITE(*,*)
1386                    WRITE(*,*) 'Hit Return When Finished Viewing'
1387                    WRITE(*,*)
1388                    READ(*,621) S
1389                    WRITE(*,*)
1390                    WRITE(*,*)
1391                    GOTO 7564
1392               ELSE IF (PRESS*101.325.LT.0.1) THEN
1393                    WRITE(*,*)
1394                   WRITE(*,*)'Current Pressure= ',PRESS*101.325,' kPa'
1395                    WRITE(*,*)
1396                    WRITE(*,*)' Error:'
1397                    WRITE(*,*)' This value is below the minimum '
1398                    WRITE(*,*)' allowable Pressure of 0.1 kPa.'
1399                    WRITE(*,*)' Raise the inlet gas pressure.'
1400                    WRITE(*,*)
1401                    WRITE(*,*) 'Hit Return When Finished Viewing'
1402                    WRITE(*,*)
1403                    READ(*,621) S
1404                    WRITE(*,*)
1405                    WRITE(*,*)
1406                    GOTO 7564
1407               ENDIF
1408  8000  CONTINUE
1409  C******END OF MAIN COMPUTATION LOOP************************************
1410
1411
1412
1413
1414  C OUTPUT OF FINAL PARAMETERS VALUES TO SCREEN AND FILE
1415  9900  CONTINUE
1416  16950 CSX = CGX * ( KC) / (KC+CONST1)
1417        TSX =TGX + HEATRX*CSX*CONST1/H
1418        IF (SSS.EQ.'I') TSX=TGX
1419        CONVX = 100.0*(CGXZ-CGX*TGX/TZERO*PZERO/PRESS)/CGXZ
1420        WRITE(*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
1421       +(CSX*1E+09/DCOSH(THIELE)),TGX,TSX,(PRESS-PZERO)*101.325
1422        WRITE(25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1423       +(CSX*1E+09/DCOSH(THIELE)),S,TGX,S,TSX,S,
1424       +(PRESS-PZERO)*101.325
1425  16900 WRITE(25,*)
```

```
1426        RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1427        WRITE(*,*)
1428        CALL HEADER(1,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1429       + DABEFF,PRESS,Y,DX)
1430        WRITE(*,*) BEEP,BEEP,BEEP
1431  17000 WRITE(*,*)
1432        WRITE(*,*) '  ==> Hit Return to Return to Main Menu <=='
1433        WRITE(*,*)
1434        READ(*,621) S
1435        WRITE(*,*)
1436        WRITE(*,*)
1437  C RESET OTHER PARAMETERS BACK TO ORIGINAL VALUES.
1438  7564     MVFLO=MVFLZ
1439           Y(1)=Y10
1440           Y(2)=Y20
1441           Y(3)=Y30
1442           Y(4)=Y40
1443           Y(5)=Y50
1444           Y(6)=Y60
1445           GOTO 9001
1446  99999 END
1447  C*****************END OF MAIN PROGRAM**********************************
1448
1449
1450
1451  C************************SUBROUTINE RK4 ******************************
1452  C-*    Programmer:  Seth Daniel Goldblum, UCSD, July 1988
1453  C-*
1454  C-*          Runge Kutta Subroutine to solve N differential
1455  C-*          Equations simultaneously.
1456  C-*
1457  C-*          This subroutine relies on a main program to feed it
1458  C-*          the following:
1459  C-*
1460  C-*          1)     The starting value of the independent variable, P
1461  C-*
1462  C-*          2)     The step size, DX
1463  C-*
1464  C-*    The subroutine returns the values of all dependent variables
1465  C-*    at the evaluated point of the independent variable in an array
1466  C-*    Xnew(N)
1467  C-*
1468  C-*    The subroutine requires and additional subroutine called func
1469  C-*    which is declared external and contains the functions of all
1470  C-*    derivatives to be evaluated simultaneously.
1471  C-*
1472  C-*          Identifiers:
1473  C-*
1474  C-*               X0(N) array of N initial values of the functions
1475  C-*               P     initial value of the independent variable
1476  C-*               F(N)  array of N elements containing the values of
1477  C-*                     the functions evaluated at some point.
1478  C-*               DX    step size
1479  C-*               XNEW(N) array of N values containing the values of
1480  C-*                     the dependent variables
1481  C-*               K1(N)  array of N values containing the values of K1
1482  C-*                     used in the Runge - Kutta method
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1483 C-*                K2(N)  array of N values containing the values of K2
1484 C-*                       used in the Runge-Kutta method
1485 C-*                K3(N)  array of N values containing the values of K3
1486 C-*                       used in the Runge - Kutta method
1487 C-*                K4(N)  array of N values containing the values of K4
1488 C-*                       used in the Runge-Kutta method
1489 C-*
1490       SUBROUTINE RK4(DX,P,X0,XNEW)
1491       REAL*8 X0(3), P, F(3), DX, XNEW(3), K1(3), K2(3), K3(3), K4(3)
1492 C-*   first approx.
1493       CALL FUNC(P,X0,F)
1494       DO 10 J=1,3
1495             K1(J)=DX*F(J)
1496             XNEW(J)=X0(J) + K1(J)/2.0
1497 10    CONTINUE
1498 c-*   second approx.
1499       CALL FUNC(DX/2.0 + P,XNEW,F)
1500       DO 20 J=1,3
1501             K2(J)=F(J)*DX
1502             XNEW(J)=X0(J) + K2(J)/2.0
1503 20    CONTINUE
1504 c-*   third approx.
1505       CALL FUNC(DX/2.0 + P, XNEW,F)
1506       DO 30 J=1,3
1507             K3(J)=F(J)*DX
1508             XNEW(J)=X0(J) + K3(J)
1509 30    CONTINUE
1510 c-*   fourth approx.
1511       CALL FUNC(DX + P,XNEW,F)
1512       DO 40 J=1,3
1513             K4(J)=F(J)*DX
1514             XNEW(J)=X0(J) + (K1(J) + 2*K2(J) +2*K3(J) +K4(J))/6.0
1515 40    CONTINUE
1516       RETURN
1517       END
1518
1519
1520
1521 C************************SUBROUTINE FUNC*********************************
1522       SUBROUTINE FUNC(P,X0,F)
1523 C-*   This subroutine is used to store the functions used
1524 C-*   in the runge-kutta method for solving them.
1525       COMMON /BLK1/ KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
1526       COMMON /BLK2/ VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
1527       REAL*8  F(3),X0(3)
1528       REAL*8 KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
1529       REAL*8 VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
1530       FGX=X0(1)
1531       TGX=X0(3)
1532 C-*   F(1) is the differential equation describing the change
1533 C-*   in molar flowrate of O2(moles/s) for a change in length:
1534       F(1) = -KC*CHSTV*MCH*MCW*(CGX-CSX)
1535 C-*
1536 C-*   F(2) is the differential equation describing the change
1537 C-*   in Pressure for a change in length
1538       F(2) = -32.0*(VISCTC/1000.0)*CHGVEL/CHHD/CHHD/101330.0
1539 C-*
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1540 C-*    F(3) is the differential equation describing the change
1541 C-*    in temperature for a change in length.
1542        F(3) = H*CHSTV*MCH*MCW/CHFLO*(TSX-TGX)/(DENGAS*CPGAS)
1543 C-*
1544        RETURN
1545        END
1546
1547
1548
1549 C**********************SUBROUTINE LINES ******************************
1550        Subroutine LINES(K)
1551        Integer      J,K
1552        DO 459 J=1,K
1553              WRITE(*,*)
1554 459    CONTINUE
1555        Return
1556        End
1557
1558
1559
1560 C**********************SUBROUTINE HEADER******************************
1561        Subroutine HEADER(FLAG,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1562       + DABEFF,PRESS,Y,DX)
1563        Real*8 PRESS,RE,CPGAS,DENGAS,CHGVEL,N,DAB,DABEFF,Y(6),DX
1564        Integer FLAG
1565        If (FLAG.EQ.0) THEN
1566              Write(*,*) ' Initial values'
1567              Write(25,*) ' Initial values'
1568        ENDIF
1569        If (FLAG.EQ.1) THEN
1570              Write(*,*) ' Final values'
1571              Write(25,*) ' Final values'
1572              WRITE(*,*)'   Mole fractions: '
1573              WRITE(*,3233) Y(1),Y(2),Y(3)
1574              WRITE(*,3234) Y(4),Y(5),Y(6)
1575              WRITE(25,*)'   Mole fractions: '
1576              WRITE(25,3233) Y(1),Y(2),Y(3)
1577              WRITE(25,3234) Y(4),Y(5),Y(6)
1578 3233         FORMAT('      He = ',F6.4,' Ar = ',F6.4,' CO2 = ',F6.4)
1579 3234         FORMAT('      CO = ',F6.4,' O2 = ',F6.4,' N2 = ',F6.4)
1580              WRITE(*,6777) PRESS*101.325
1581 6777         FORMAT('   Gas Pressure (kPa):            ',F9.3)
1582              WRITE(25,6777) PRESS*101.325
1583        ENDIF
1584        WRITE(*,10) RE
1585 10     Format('   Reynolds number =            ',F9.3)
1586        WRITE(*,20) CPGAS
1587 20     Format('   Gas Heat Capacity (J/K-g) =  ',F9.3)
1588        WRITE(*,30) DENGAS*1000
1589 30     Format('   Gas Density (g/cm^3) =          ',F10.7)
1590        WRITE(*,40) CHGVEL
1591 40     Format('   Gas Velocity (mm/s) =        ',F9.3)
1592        WRITE(*,50) N
1593 50     Format('   Effectivness factor =          ',F9.5)
1594        WRITE(*,60) DAB/100.0
1595 60     Format('   Bulk Gas Diffusivity(cm^2/s)=  ',F9.5)
1596        WRITE(*,70) DABEFF/100.0
```

```
1597  70    Format('   Effective Diffusivity(cm^2/s)=  ',F9.6)
1598        WRITE(*,80) DX
1599  80    Format('   Step size(mm) =                 ',F9.6)
1600        WRITE(25,10) RE
1601        WRITE(25,20) CPGAS
1602        WRITE(25,30) DENGAS*1000
1603        WRITE(25,40) CHGVEL
1604        WRITE(25,50) N
1605        WRITE(25,60) DAB/100
1606        WRITE(25,70) DABEFF/100
1607        WRITE(25,80) DX
1608        Return
1609        End
1610
1611
1612
1613  C**********************SUBROUTINE TCON ******************************
1614        Subroutine TCON(T,TCONT)
1615        Real*8       T,TCONT(6)
1616  C     Compute thermal cond.(TCONT(i)) for a given species at temp. T
1617  C     Units on TCON are mW/cM-K.
1618  C     The index of TCONT(i) corresponds to the species.
1619  C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1620  C     The following polynomial equations used to compute the
1621  C     thermal conductivity of each species at temperature T
1622  C     have been taken from page 515 of "Properties of Gases and Liquids"
1623  C     4th Ed. Reid, Prausnitz, & Sherwood
1624        TCONT(1) = (3.722E-2 + 3.896E-4*T - 7.450E-8*T**2 +
1625       1   1.290E-11*T**3)*10.0
1626        TCONT(2) = (2.714E-3 + 5.540E-5*T - 2.178E-8*T**2 +
1627       1   5.528E-12*T**3)*10.0
1628        TCONT(3) = (-7.215E-3 + 8.015E-5*T + 5.477E-9*T**2 -
1629       1   1.053E-11*T**3)*10.0
1630        TCONT(4) = (5.067E-4 + 9.125E-5*T - 3.524E-8*T**2 +
1631       1   8.199E-12*T**3)*10.0
1632        TCONT(5) = (-3.273E-4 + 9.966E-5*T - 3.743E-8*T**2 +
1633       1   9.732E-12*T**3)*10.0
1634        TCONT(6) = (3.919E-4 + 9.816E-5*T - 5.067E-8*T**2 +
1635       1   1.504E-11*T**3)*10.0
1636        Return
1637        End
1638
1639
1640
1641  C**********************SUBROUTINE PROP ****************************
1642        Subroutine PROP(Y,TCONT,VISCT,VISCTC,K)
1643        Real*8       AX(6,6),VISCTC,K,SUM,MW(6),Y(6),TCONT(6)
1644        Real*8       CONSTE,CONSTD,VISCT(6),LAMBMX,CONSTF
1645        Integer      I,J
1646  C     Read in molecular weights MW(I) into array.
1647  C     The index of MW correspond to the species.
1648  C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1649        DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1650       +     / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1651  C     Compute parameter matrix AX(i,j)
1652  C     The indexes of A(i,j) correspond to the species.
1653  C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
```

```
1654 C The AX(i,j) matrix is defined on p. 531 of "Properties of Gases and
1655 C Liquids", 4TH ed.,Reid, Prausnitz,& Sherwood. Both the bulk gas
1656 C thermal conductivity and the bulk gas viscosity can be computed
1657 C using the AX(6,6) matrix.
1658       VISCTC = 0.0
1659       LAMBMX=0.0
1660       DO 551 I =1,6
1661             SUM = 0.0
1662             DO 651 J = 1,6
1663                   IF(I.EQ.J) THEN
1664                         AX(I,J)=1.0
1665                   ELSE
1666                         CONSTE = MW(I)/MW(J)
1667                         CONSTD = VISCT(I)/(CONSTE*VISCT(J))
1668                         CONSTD = DSQRT(CONSTD)
1669                         AX(I,J) = (1+CONSTD*CONSTE**0.25)**2/
1670      *                                DSQRT(8.0*(1.0+CONSTE))
1671                   END IF
1672                   SUM = SUM + Y(I)*AX(I,J)
1673 651         CONTINUE
1674             CONSTF = Y(I) / SUM
1675             LAMBMX = LAMBMX + CONSTF*TCONT(I)
1676             VISCTC = VISCTC + CONSTF*VISCT(I)
1677 551   CONTINUE
1678       K = LAMBMX/10000.0
1679       RETURN
1680       END
1681
1682
1683
1684 C**********************SUBROUTINE VIS ******************************
1685       Subroutine VIS(T,VISC,VISCT)
1686       Real*8      T,VISC(6,2:7),VISCT(6),CONST5
1687       Integer     I
1688 C     Compute viscosity (VISCT(i)) for a given species at temp. T
1689 C     Units on VISCT are centipoises.
1690 C     The index of VISC corresponds to the species.
1691 C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1692 C     CONST5 is a temporary value holding constant
1693       DO 2223 I=1,6
1694             CONST5=VISC(I,INT(1+T/100.0))-VISC(I,INT(T/100.0))
1695             CONST5=CONST5*(T/100.0-INT(T/100.0))
1696             VISCT(I)=VISC(I,INT(T/100.0)) + CONST5
1697 2223  CONTINUE
1698       RETURN
1699       END
1700
1701
1702
1703 C**********************SUBROUTINE OUTPUT*****************************
1704       Subroutine OUTPUT(FLAG,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
1705      +            Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
1706      +            EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
1707      +            CONV,MONOL,DX,CDI)
1708       Integer     FLAG
1709       Real*8      MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT
1710       Real*8      Y(6),MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT
```

```
      Real*8       EMICRO,EMACRO,RMICRO,RMACRO
      Character*1 SSS,SSS1,SSS2,S
      Real*8       CONV,MONOL,DX,CDI
C  Flag=0 => Output parameters to screen for review
C  Flag=1 => Output parameters to file LDATA
      IF (FLAG.EQ.1)    GOTO 40000
      Write(*,6000)
6000  FORMAT(20X,'       SELECTABLE PARAMETER SUMMARY')
      WRITE(*,*)' Monolith Dimensions(mm): '
      WRITE(*,6001) MCST*2,MFDH,MFDV
6001  FORMAT(' Support wall thickness: ',F6.2,3X,'Face dimension: ',
     2F7.2,' x ',F7.2)
      WRITE(*,6002) MCW,NOCHV,NOCHH
6002  FORMAT(' Channel inner dimension:',F6.2,3X,'No.Face channels',
     2': ',F6.2,'   x  ',F6.2)
      WRITE(*,6003) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
6003  FORMAT(' Active layer thickness:',F6.2,4x,'% monol.volume',
     +' open : ', F6.1)
      WRITE(*,*)
      WRITE(*,*)' Monolith inlet parameters:'
      WRITE(*,6006) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
6006  FORMAT(' Gas Composition (mole fraction):    CO2: ',F6.4,2X,
     2'CO: ',F6.4,2X,'O2: ',F6.4,/,38X,'N2: ',F6.4,2X,'He: ',F6.4,2X,
     3'Ar: ',F6.4)
      WRITE(*,6007) MVFLZ,TZERO,PZERO*101.325
6007  FORMAT(' Gas Flowrate(liters/s):',F7.3,'  Gas Temperature(K): ',
     2F7.2/  ' Inlet Gas Pressure (kPa): ',F9.3)
      WRITE(*,*)
      WRITE(*,*)' Catalyst Properties:'
      WRITE(*,6008) DENCAT
6008  FORMAT(' Catalyst Density (g/mm^3):',E10.3)
      WRITE(*,6009) AREF
6009  FORMAT(' Reaction rate constant at 298K(mm^3 /gcat-s): ',F8.2)
      WRITE(*,6010) ENGACT
6010  FORMAT(' Activation energy(J/mol): ',F10.2)
      WRITE(*,6004)EMICRO,EMACRO
6004  FORMAT(' Void-fraction as micropores: ',F4.2,
     2       '   Void-fraction as macropores: ',F4.2)
      WRITE(*,6005)RMICRO,RMACRO
6005  FORMAT(' Avg. micropore radius (nm): ',E7.2,
     2       ' Avg. macropore radius (nm): ',E7.2)
      IF (SSS.EQ.'A')   WRITE(*,6011)
6011  FORMAT(' Thermal Operation (adiabatic/isothermal): Adiabatic')
      IF (SSS.EQ.'I')   WRITE(*,6012)
6012  FORMAT(' Thermal Operation (adiabatic/isothermal): Isothermal')
      WRITE(*,*)
      WRITE(*,*)' Computational loop parameters:'
      IF (SSS1.EQ.'S')  WRITE(*,6013)
6013  FORMAT(' Output file (Full Profile/Summary): Summary')
      IF (SSS1.EQ.'P')  WRITE(*,6014)
6014  FORMAT(' Output file (Full Profile/Summary): Full Profile')
      IF (SSS2.EQ.'O')  WRITE(*,6015) CONV
6015  FORMAT(' Termination on (O2 conversion/Length): ',
     2'O2 conversion.  %: ', F7.3)
      IF (SSS2.EQ.'L')  WRITE(*,6016) MONOL
6016  FORMAT(' Termination on (O2 conversion/Length): ',
     2'Length.  Length(mm): ', F7.3)
```

```
1768        IF (SSS1.EQ.'P') WRITE(*,6017) DX,CDI
1769  6017  FORMAT(' Computation loop step size(mm): ',F7.4,
1770       2'   Display every ',F6.2,' mm')
1771        IF (SSS1.EQ.'S') WRITE(*,6018) DX
1772  6018  FORMAT(' Computation loop step size(mm): ',F7.4)
1773        WRITE(*,*)
1774        WRITE(*,6019)
1775  6019  FORMAT(15X,'   ==> Hit Return When Finished Viewing <==')
1776  621   FORMAT(A)
1777        READ(*,621) S
1778        WRITE(*,*)
1779        WRITE(*,*)
1780        GOTO 80000
1781  40000 WRITE(*,*)'              *****SEE FILE LDATA FOR RESULTS*****'
1782        WRITE(25,*)
1783        WRITE(25,6000)
1784        WRITE(25,*)' Monolith Dimensions(mm): '
1785        WRITE(25,6001) MCST*2,MFDH,MFDV
1786        WRITE(25,6002) MCW,NOCHV,NOCHH
1787        WRITE(25,6003) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
1788        WRITE(25,*)
1789        WRITE(25,*)' Monolith inlet parameters:'
1790        WRITE(25,6006) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
1791        WRITE(25,6007) MVFLZ,TZERO,PZERO*101.325
1792        WRITE(25,*)
1793        WRITE(25,*)' Catalyst Properties:'
1794        WRITE(25,6008) DENCAT
1795        WRITE(25,6009) AREF
1796        WRITE(25,6010) ENGACT
1797        WRITE(25,6004)EMICRO,EMACRO
1798        WRITE(25,6005)RMICRO,RMACRO
1799        IF (SSS.EQ.'A')   WRITE(25,6011)
1800        IF (SSS.EQ.'I')   WRITE(25,6012)
1801        WRITE(25,*)
1802        WRITE(25,*)' Computational loop parameters:'
1803        IF (SSS1.EQ.'S')  WRITE(25,6013)
1804        IF (SSS1.EQ.'P')  WRITE(25,6014)
1805        IF (SSS2.EQ.'O')  WRITE(25,6015) CONV
1806        IF (SSS2.EQ.'L')  WRITE(25,6016) MONOL
1807        IF (SSS1.EQ.'P')  WRITE(25,6017) DX,CDI
1808        IF (SSS1.EQ.'S')  WRITE(25,6018) DX
1809        WRITE(25,*)
1810        WRITE(*,*)
1811  80000 RETURN
1812        END
1813
1814
1815
1816  C****************  FUNCTION FXN1      ********************
1817        FUNCTION FXN1(TDAB,Y5,PRESS,RMICRO,RMACRO,
1818       + TSX,EMACRO,EMICRO)
1819        REAL*8 TDAB,Y5,PRESS,RMICRO,RMACRO
1820        REAL*8 TSX,EMACRO,EMICRO,DKMICR,DKMACR
1821        REAL*8 DMACRO,DMICRO
1822  C     Effective diffusivity is computed using the micro-macro
1823  C     pore model of Wakao and Smith as described on pages 170-
1824  C     171 of Chemical Reactor Analysis and Design by Froment
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1825 C      and Bishoff
1826        TDAB=(1-Y5)/TDAB/PRESS
1827        DKMICR =171482.0*RMICRO/1E+7*DSQRT(TSX)
1828        DKMACR =171482.0*RMACRO/1E+7*DSQRT(TSX)
1829        DMICRO =1.0/(1.0/TDAB + 1.0/DKMICR)
1830        DMACRO =1.0/(1.0/TDAB + 1.0/DKMACR)
1831        FXN1 = EMACRO**2*DMACRO + (EMICRO**2*DMICRO*(1.0 +
1832       *         3.0*EMACRO))/(1.0 - EMACRO)
1833        RETURN
1834        END
1835
1836
1837
1838 C****************** FUNCTION FXN2      ********************
1839        Function FXN2(Y,TGX)
1840 C      Function computes heat capacity of gas mixture using data
1841 C      from the JANAF tables.
1842 C      MW,CP,Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 5=O2, 6=N2
1843        Real*8 Y(6),TGX,CP(6),MW(6)
1844 C      Read in molecular weights MW(I) into array.
1845        DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1846       +     / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1847        CP(1)=20.786
1848        CP(2)=20.786
1849        CP(3)=20.712+6.2501E-02*TGX-1.188E-5*TGX*TGX
1850       +      -5.5773E-08*TGX*TGX*TGX + 4.1875E-11*TGX*TGX*TGX*TGX
1851        CP(4)=28.777  +  5.5297E-03*TGX  -3.1851E-5*TGX*TGX
1852       +     +7.0946E-08*TGX*TGX*TGX  -4.2501E-11*TGX*TGX*TGX*TGX
1853        CP(5)=31.033  -  2.0261E-02*TGX  +6.3410E-5*TGX*TGX
1854       +     -4.9951E-08*TGX*TGX*TGX +9.1266E-12*TGX*TGX*TGX*TGX
1855        CP(6)=28.567  +  7.3978E-03*TGX  -3.5831E-05*TGX*TGX
1856       +     +6.9415E-08*TGX*TGX*TGX -3.8499E-11*TGX*TGX*TGX*TGX
1857        FXN2 =  Y(1)*CP(1)/MW(1) + Y(2)*CP(2)/MW(2) +
1858       +        Y(3)*CP(3)/MW(3) + Y(4)*CP(4)/MW(4) +
1859       +        Y(5)*CP(5)/MW(5) + Y(6)*CP(6)/MW(6)
1860        RETURN
1861        END
1862
1863
1864
1865 C**********************FUNCTION FXN3*********************************
1866        Function FXN3(Y,TGX)
1867        Real*8      Y(6),D(6),TGX,CONST
1868 C      Compute diffusivity of O2 in gas mixture
1869 C      Read in binary diffusion coefficients D(I) into array.
1870 C      The index of D correspond to the species in which O2 is diffusing
1871 C      Note: There is no D(5) defined. These are reference values at
1872 C            298K, 1 atm, units(mm^2/s)
1873 C      Species: 1=He,2=Ar,3=CO2,4=CO,6=N2.
1874        DATA D(1),D(2),D(3),D(4),D(6)
1875       +     /72.9,21.2,16.4,15.6,22.5/
1876        CONST=0.0
1877        DO 8451 I=1,6
1878              IF (I.EQ.5) GO TO 8451
1879              CONST= Y(I)/(D(I)*(TGX/298.0)**1.5)+CONST
1880 8451   CONTINUE
1881        FXN3=CONST
```

```
1882        RETURN
1883        END
1884
1885
1886
1887  C**********************FUNCTION FXN4*********************************
1888        Function FXN4(Y)
1889        Real*8 MW(6),Y(6),CONST
1890  C     Compute gas average molecular weight
1891  C     MW,Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 5=O2, 6=N2
1892  C     Read in molecular weights MW(I) into array.
1893  C     The index of MW correspond to the species.
1894  C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1895        DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1896       +     / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1897        CONST=0.0
1898        DO 355 I=1,6
1899             CONST=MW(I)*Y(I)+CONST
1900  355   CONTINUE
1901        FXN4=CONST
1902        RETURN
1903        END
1904
1905
1906  C*************            END OF LISTING        **********************
1907
```